



Weierstrass Institute for Applied Analysis and Stochastics



Intelligent solutions for complex problems

Annual Research Report 2006

Cover figure: Temporal axial distribution of field intensity in a three-section semiconductor laser operating in chaotic state.

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The Weierstrass Institute for Applied Analysis and Stochastics (WIAS, member of the Leibniz Association) presents its Annual Report 2006. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2006. Following a more general introduction in part one, in its second part five selected scientific contributions, written for a broader public, highlight some results of outstanding importance. Finally, the third part presents the essential results of the research groups.

The year 2006 was marked by an audit in March in which the Scientific Advisory Board evaluated the institute. We passed this examination with distinction. The work in the *Research Program 2004–2006* continued successfully, and WIAS further consolidated its leading position in the mathematical community as a center of excellence in the treatment of complex applied problems. Several scientific breakthroughs were achieved, some of which will be detailed later in this report, and WIAS has even expanded its scope into new applied problems from medicine, economy, science, and engineering, especially in its main fields of competence:

- Nano- and optoelectronics
- Optimization and control of technological processes
- Phase transitions and multifunctional materials
- Stochastics in science and economics
- Flow and transport processes in continua
- Numerical methods of analysis and stochastics

The positive development is reflected by the successful acquisition of grants, by the number of international workshops organized by the institute, by numerous invited lectures held by WIAS members at international meetings and research institutions, and by the many renowned foreign visitors hosted by the institute last year.

The number of refereed journal publications increased by nearly 25% compared to 2005, a remarkable success, and the best result ever. In addition to this, six excellent monographs authored or edited by WIAS members appeared in renowned scientific series of top-selling publishing companies. Each one of these monographs marks a milestone and culmination point of long-standing research at WIAS, and is visible evidence for the scientific excellence of its collaborators.

As another highlight of 2006, Prof. Anton Bovier, the second Deputy Director of WIAS, delivered a lecture at the International Congress of Mathematicians 2006 in Madrid; he was one of only eight German speakers at this World Congress. Also at the ICM 2006, the WIAS director Prof. Jürgen Sprekels became one of the two coordinators of the International Mathematical Sciences Institutes (IMSI).

The high rank of WIAS in the mathematical community is also witnessed by the fact that the year-long success story of “Transfer of knowledge via brains” through the institute’s members continued also in 2006: Dr. Barbara Gentz was appointed W2 Professor for Probability Theory at the University of Bielefeld, and Dr. Christian Bender left WIAS for a Junior Professorship at the Technical University of Braunschweig. Since the institute’s foundation in 1992, a total of 33 calls (including 16 to full professorships in Germany and nine to professorships abroad) have been received by



*Prof. Dr. Jürgen Sprekels,
Director*

WIAS members; given the fact that presently there are 54 scientists on the budget of WIAS, this is a truly remarkable output of which we are proud. Also remarkable is the fact that since 2003 no less than three female members of WIAS have been called to university professorships.

2006 has again been a “year of workshops” at WIAS. Nine international workshops organized by WIAS evidenced the institute’s reputation and its role as an attractive meeting place for international scientific exchange and cooperation. In addition to this, WIAS members (co-) organized numerous scientific meetings throughout the world; in particular, PD Dr. Barbara Wagner was one of the organizers of a conference at the Mathematisches Forschungsinstitut Oberwolfach (MFO). Also the guest program of WIAS was intensified in 2006 by hosting the first winners of the Weierstrass Postdoctoral Fellowships (see page 125).

In addition to these “global” activities, WIAS has on the “local” scale intensified its well-established cooperation with the other mathematical institutions in Berlin, with the main attention directed toward the three Berlin universities. This is witnessed by the fact that as of today five leading members of WIAS, including the director and his two deputies, hold special chairs funded by WIAS at the Berlin universities. Another such appointment is under way, and we are hoping that by the end of 2007 six WIAS members will hold chairs funded by WIAS at the Berlin universities.

The highlight of cooperation with the mathematical institutions in Berlin was also in 2006 the joint operation of the DFG Research Center MATHEON “Mathematics for key technologies” located at the Technical University of Berlin. In January 2006, MATHEON was evaluated by an international panel of referees and passed with distinction. As consequence, the Center was granted a second funding period until May 2010, and DFG funds exceeding 5.5 million euros per year will continue to flow into Berlin for MATHEON to become an international beacon of applied mathematics. WIAS is committed to the success of the Center by providing considerable financial and personal resources: the Director of WIAS is a member of MATHEON’s Executive Board, both his deputies are “Scientists in Charge” of mathematical fields in the center, and members of WIAS participate in the management of 18 of its subprojects. In turn, in 2006 up to 14 scientific collaborators and several student assistants employed at WIAS were funded by MATHEON.

Another big success story for the mathematical community of Berlin was the successful application for the “Berlin Mathematical School” (BMS) in the framework of the German “Competition for Excellence”. The BMS, a graduate school for advanced mathematical studies, will bring together the capacities of all mathematical institutions in Berlin to attract excellent doctoral students from all over the world. Also in this application, members of WIAS took part as principal investigators, and many members of WIAS will serve in the BMS, teaching courses and supervising doctoral students.

Besides these major activities, and besides the cooperation with the universities through the manifold teaching activities of its members, WIAS initiated and participated in successful applications for Collaborative Research Centers, Priority Programs, and Research Training Groups of the German Research Foundation (DFG). For example, the institute contributes considerably to the operation of the DFG Research Training Group “Analysis, Numerics, and Optimization of Multiphase Problems” at the Humboldt-Universität zu Berlin, and Prof. Anton Bovier, the second Deputy Director of WIAS, is the Speaker of the newly-founded International DFG Research Training Group “Stochastic Models

of Complex Processes”, which combines groups from the Technical and the Humboldt University, WIAS, and the University of Potsdam, with groups from the University of Zurich and the ETH Zurich.

Our primary aim remains unchanged: to join fundamental research with application-oriented research, and, by new scientific insights, to contribute to the advancement of innovative technologies. The recent achievements give evidence that this concept, in combination with hard, continuing work in scientific details, eventually leads to success.

We hope that funding agencies, colleagues, and partners from industry, economy, and sciences will find this report informative and will be encouraged to cooperate with us.

Berlin, in March 2007

J. Sprekels

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1 WIAS in 2006

- Profile
- Structure and Scientific Organization
- Grants



1.1 Profile

The *Weierstrass Institute for Applied Analysis and Stochastics* (Weierstraß-Institut für Angewandte Analysis und Stochastik, WIAS) is part of the *Forschungsverbund Berlin e.V. (FVB)*. FVB is a legal entity in which eight scientifically independent member institutes of the *Leibniz Association* are combined. The *Director of WIAS* is responsible for the scientific work at WIAS, the *Manager of the Common Administration of FVB* is in charge of its administrative business.

The mission of WIAS is to carry out *project-oriented* research in applied mathematics. WIAS contributes to the solution of complex economic, scientific, and technological problems of supranational interest; its research is interdisciplinary and covers the entire process of problem solution, from modeling to the mathematical analysis of the models, to the development and implementation of efficient and robust algorithms, and the simulation of technological processes. In its field of competence, WIAS plays a leading role in Germany and worldwide.

WIAS promotes the international cooperation in applied mathematics by organizing workshops and running guest and postdoc programs. A special emphasis is devoted to the extension of the institute's traditional contacts to the scientific institutions of Eastern Europe.

A successful mathematical approach to complex applied problems necessitates a long-term multiply interdisciplinary cooperation in project teams. Besides maintaining the contact to the customers from the applications, which means, in particular, to master their respective technical terminologies, the WIAS members have to combine their different mathematical expertises and programming skills. This interdisciplinary teamwork takes full advantage of the possibilities provided in a research institute. It also advances the internal scientific networking and helps optimize the common efforts of the institute's scientific staff.

1.2 Structure and Scientific Organization

1.2.1 Structure

To fulfill its mission, WIAS is presently structured in departments for technical services and the seven scientific research groups¹

RG 1. Partial Differential Equations

RG 2. Laser Dynamics

RG 3. Numerical Mathematics and Scientific Computing

RG 4. Nonlinear Optimization and Inverse Problems

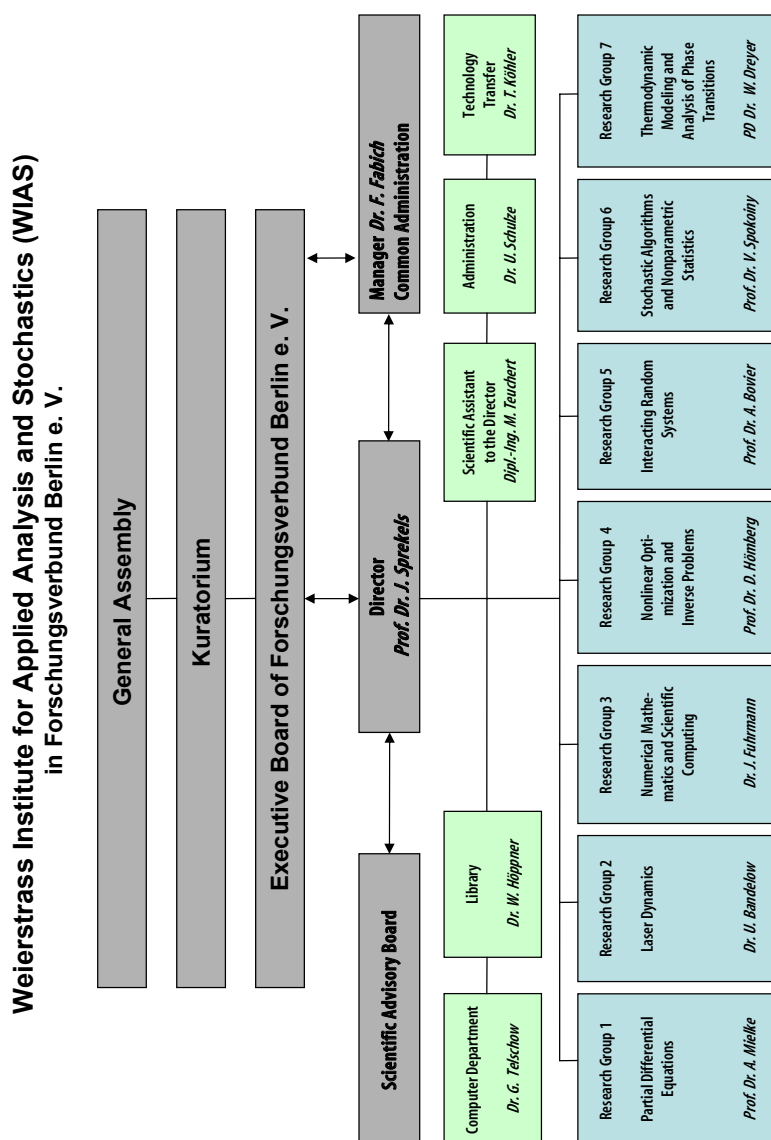
RG 5. Interacting Random Systems

RG 6. Stochastic Algorithms and Nonparametric Statistics

RG 7. Thermodynamic Modeling and Analysis of Phase Transitions

¹In the following, the term "research group" will often be abbreviated by "RG".

The following organization chart gives an overview of the organizational structure:



1.2.2 Main Fields of Research

The research at WIAS is presently focusing on the following *main fields*, in which the institute has an outstanding competence in modeling, analysis, and simulation:

- **Nano- and optoelectronics**
- **Optimization and control of technological processes**
- **Phase transitions and multifunctional materials**
- **Stochastics in science and economics**
- **Flow and transport processes in continua**
- **Numerical methods of analysis and stochastics**

To these fields, WIAS has made important contributions in the past years that strongly influenced the directions of development of worldwide research. The institute has a special modeling and simulation expertise in two promising modern technologies:

- Optical technologies (in particular, diffractive and laser structures, optical fibers)
- Fuel cells (direct methanol fuel cells)

1.2.3 Contributions of the Research Groups of WIAS

The seven research groups form the institute's basis to fully bring to bear and develop scope and depth of its expertise. The mathematical problems studied by the research groups originate both from short-term requests arising during the solution process of real-world problems, and from the continuing necessity to acquire further mathematical competence as prerequisite to enter new fields of applications. This necessitates a well-directed long-term *basic research in mathematics*.

The following table gives an overview to which main fields the research groups have contributed in 2006 in the interdisciplinary solution process described above.

Main Fields	RG 1	RG 2	RG 3	RG 4	RG 5	RG 6	RG 7
Nano- and optoelectronics	*	*	*	*	—	—	—
Optimization and control of technological processes	—	—	*	*	—	*	*
Phase transitions and multifunctional materials	*	—	*	*	*	—	*
Stochastics in science and economics	—	—	*	*	*	*	*
Flow and transport processes in continua	*	—	*	—	*	*	*
Numerical methods of analysis and stochastics	*	*	*	*	*	*	*

In the following, we list special research topics that have been addressed in 2006 within the general framework of the main fields. The research groups that have contributed to the respective studies are indicated in brackets.

1. Nano- and optoelectronics

- Technology and device simulation of semiconductor devices (in RG 1 and RG 3)
- Phenomenological modeling of semiconductor heterostructures (in RG 1)
- Diffractive optics (simulation and optimization of optical gratings; in RG 4)
- Quantum mechanical modeling of nanostructures (in RG 1 and RG 3)
- Laser structures (in RG 1 and RG 2)

2. Optimization and control of technological processes

- Simulation and control in process engineering (in RG 3 and RG 4)
- Virtual production planning (optimization and inverse modeling of multibody systems; in RG 3 and RG 4)
- Problems of Optimal Shape Design (in RG 4 and RG 7)
- Optimal control of heat treatments and milling processes (in RG 4 and RG 7)

3. Phase transitions and multifunctional materials

- Modeling of nonlinear phenomena and phase transitions in multifunctional materials (hysteresis in shape memory alloys and piezo effects in ferromagnetic and ferroelectric materials; in RG 1 and RG 7)
- Thermomechanical modeling of phase transitions in steels (in RG 4 and RG 7)
- Modeling and simulation of gas–liquid and liquid–solid transitions, phase separation with thermomechanical diffusion (Stefan problems, phase field models, LSW theory, Becker–Döring models; in RG 7)
- Stochastic modeling of phase transitions (in RG 5)
- Growth of semiconductor bulk single crystals (silicon carbide, aluminum nitride, gallium arsenide; in RG 7)

4. Stochastics in science and economics

- Stochastic particle systems and kinetic equations (modeling and simulation of coagulation processes and gas flows; in RG 5, RG 6, and RG 7)
- Modeling of stock prizes, interest rates, and exchange rates (in RG 5 and RG 6)
- Evaluation of derivatives, portfolio management, and evaluation of risk (in RG 6)
- Nonparametric statistical methods (image processing, financial markets, econometrics; in RG 6)
- Dynamical processes in nonhomogeneous media (in RG 5 and RG 7)

5. Flow and transport processes in continua

- Treatment of Navier–Stokes equations (in RG 3 and RG 7)
- Flow and mass exchange in porous media (water and materials transport in soils and in porous rocks, two-phase flows; in RG 3)
- Modeling of fuel cells (in RG 3)
- Modeling of nanostructures of thin films on crystalline surfaces (in RG 7)

6. Numerical methods of analysis and stochastics

- Numerical solution of partial differential equations (finite volume and finite element methods, preconditioners, grid generation, error estimators, and adaptivity; in all research groups, especially in RG 3)
- Numerics of inverse problems (integral equations, regularization techniques; in RG 1, RG 4, and RG 6)
- Nonlinear optimization techniques (in RG 4)
- Stochastic numerics (Monte Carlo methods, kinetic equations, coagulation dynamics, particle systems; in RG 5, RG 6, and RG 7)
- Development of WIAS software packages (AWS, BOP, ClusCorr98, DiPoG, glttools, LDSL-tool, pdelib2, TetGen, WIAS-HiTNIHS, WIAS-MatConE, WIAS-SHarP, WIAS-TeSCA, WIAS-QW, ...)

1.3 Grants

The raising of grants under scientific competition is one of the main indicators of scientific excellence and thus plays an important role in the efforts of WIAS. In this task, WIAS has been quite successful in 2006, having raised a total of 1.535 million euros, from which additional 28 researchers (Dec. 31, 2006) have been financed. Particularly important is the fact that the funds raised in industrial collaborations could be kept at 268,000 euros. In total, 25.53 per cent of the total budget of WIAS in 2006, and 32.95 per cent of its scientific staff, originated from grants. In the following, some projects of particular interest and importance will be highlighted, without going into too much detail².

1.3.1 DFG Research Center MATHEON

The highlight of cooperation with the mathematical institutions in Berlin has been the joint operation of the DFG Research Center MATHEON “Mathematics for key technologies”. Following a very successful evaluation by an international panel of referees in January 2006, MATHEON was granted

²For a detailed account of projects funded by third parties, we refer the reader to the appendix, Section A.2 Grants below.

a second funding period until 2010. Annually, DFG funds exceeding 5.5 million euros flow into Berlin for MATHEON. WIAS dedicates considerable financial and personal resources to the Center: its director is a member of MATHEON's Executive Board, both his deputies are "Scientists in Charge" of mathematical fields in the Center, and members of WIAS participate in the management of 18 of its subprojects. In turn, in 2006 up to 14 scientific collaborators and several student assistants at WIAS were funded by MATHEON.

1.3.2 Graduate School *Berlin Mathematical School (BMS)*

Berlin's mathematicians won this graduate school, which is run by the three major Berlin universities, within the framework of the German Initiative for Excellence last year in a joint effort. Funds exceeding one million euros per year for the BMS, which started operations in the fall of 2006, will for five years strengthen the efforts of the mathematical institutions of Berlin to attract excellent young PhD students to the city. Among the principal investigators of this successful initiative have been both Deputy Directors of WIAS, Profs. A. Bovier (RG 5) and A. Mielke (RG 1). Many further members of WIAS will contribute to the future operations of the BMS.

1.3.3 International Research Training Group *Stochastic Models of Complex Processes of the DFG*

The acquisition of this international graduate college, which is operated jointly with ETH Zürich and University of Zurich, Switzerland, has been another big success of the activities of Berlin's mathematicians in 2006. The graduate college, whose first funding period runs from July 2006 to December 2011, is located at the Technical University of Berlin; its Coordinator is Prof. A. Bovier, the second Deputy Director of WIAS.

1.3.4 DFG Research Training Group GRK 1128 *Analysis, Numerics, and Optimization of Multiphase Problems*

In the Research Training Group GRK 1128 at Humboldt-Universität zu Berlin, which started operations in April 2005 (first funding period: until September 2009), a number of WIAS members are active as principal investigators and associate members; Prof. D. Hömberg (RG 4) has been its Deputy Coordinator in 2006. WIAS members are presently supervising the theses of four graduates.

1.3.5 Krist^WMAG

In this research project, which is being funded since July 2005 in the "Zukunftsfonds" of the state of Berlin and headed by the Institute of Crystal Growth in Berlin-Adlershof, WIAS cooperates with several industrial companies and other research institutions. The project aims at the development of a new technique for the crystal growth from a melt under the impact of magnetic fields.

1.3.6 BMBF Project *Numerical simulation for direct methanol micro fuel cells*

This research project, which started operations in 2005 and will run until June 2008, is funded by the German Ministry of Education and Research in the framework of the funding program "Networks for Basic Research in Renewable Energies and Energy Efficiency". It is part of an interdisciplinary joint project for the experimental investigation, modeling, and numerical simulation of direct methanol micro fuel cells, which is coordinated by the acting head of RG 3, Dr. J. Fuhrmann.

2 Scientific Highlights

- Continuum Description of Discrete Lattice Models
- Optimization Problems with Random Constraints
- Creating Novel Devices for High-speed Optical Telecommunications
- Three-dimensional Boundary Conforming Delaunay Mesh Generation — The TetGen Project
- Applied Mathematical Finance: Iterating Cancelable Snowballs and Related Exotic Products

2.1 Continuum Description of Discrete Lattice Models

Wolfgang Dreyer and Alexander Mielke

Motivations and objectives

From a mathematical point of view, lattice models consist of an initial value problem for a large system of N ordinary differential equations (ODE). Here, the main objective is a study of limiting cases $N \rightarrow \infty$ that allow us to substitute the discrete ODE system by a single or at most a few partial differential equations (PDE) that describe the discrete dynamics on a continuum level. Among the challenges in this field are the following general questions for multiscale problems:

- How many features of the ODE system survive on the continuum scale?
- What microscopic averages can be effectively described by macroscopic PDEs?
- What microscopic structures can be recovered by solving the PDEs?

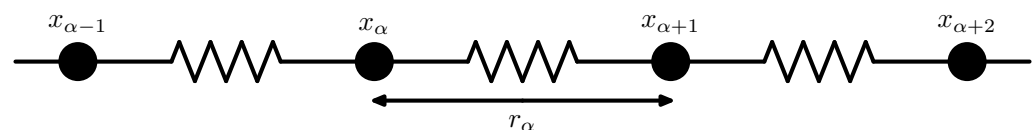
In physics, lattice models serve as simple models that allow us to simulate the dynamics of *macroscopic* bodies, say solids, on an atomistic scale, where their *microscopic* discrete structure is described by structureless atoms that all interact with each other by given forces. In this setting, the ODE system is given by NEWTON's equation of motion for N atoms. Here, one expects that possible limiting cases $N \rightarrow \infty$ lead to a small PDE system for macroscopic quantities within the framework of the laws of thermodynamics.

In this article, we will focus on some selected aspects of these problems. In particular, we will show that the limit $N \rightarrow \infty$ must be simultaneously carried out by a corresponding scaling of time and space. However, this can be done in various ways, leading to different PDE systems.

Special lattice models

The simplest lattice model is given by an atomic chain in one space dimension, which consists of N atoms, described as structureless particles with nearest-neighbor interactions. The particles have the same mass m , they are indexed by α , and at time t they are located at positions $x^\alpha(t)$. Various boundary conditions are possible. For example, a periodic chain that conserves total momentum and total energy is described by $r_0(t) = r_N(t)$ and $v_{N+1}(t) = v_1(t)$. For RIEMANN problems, other types of boundary conditions are more appropriate, see [4] for more details.

Fig. 1: The atomic chain with nearest-neighbor interactions



The basic variables are the distances $r_\alpha(t) = x_{\alpha+1}(t) - x_\alpha(t)$ and the velocities $v_\alpha(t) = \dot{x}_\alpha(t)$. The microscopic dynamics of the atomic chain is determined by NEWTON's equation of motion, which reads in conservative form

$$r_\alpha = v_{\alpha+1} - v_\alpha, \quad v_\alpha = \Phi'(r_{\alpha+1}) - \Phi'(r_\alpha). \quad (1)$$

The interaction potential Φ contains repulsive parts if particles come close to each other, and attracting parts for larger distances.

More general lattice systems occur in higher space dimensions. For simplicity, we assume that we have the infinite periodic lattice \mathbb{Z}^d of all points with integer coordinates in d space dimensions. Each lattice point $\alpha \in \mathbb{Z}^d$ corresponds to a group of possibly different atoms (e.g., in an alloy) whose positions are collected in the vector $x_\alpha \in \mathbb{R}^m$. NEWTON's equation takes the form

$$M\ddot{x}_\alpha = -\nabla_x V_0(x_\alpha) - \sum_{0 < |\beta| \leq R} \left(\nabla_x V_\beta(x_\alpha - x_{\alpha+\beta}) - \nabla_x V_\beta(x_{\alpha-\beta} - x_\alpha) \right), \quad (2)$$

where $M \in \mathbb{R}^{m \times m}$ is a positive definite mass matrix, V_0 denotes an on-site potential, and V_β are the interaction potentials. $R > 1$ provides a threshold beyond which the interactions are neglected.

For several physical aspects, like propagation of phonons, it is even enough to study the linear version of equation (2), namely

$$M\ddot{x}_\alpha = - \sum_{0 \leq |\beta| \leq R} A_\beta x_{\alpha+\beta}, \quad (3)$$

as it can be studied in great detail via Fourier transformation methods. In particular, one can construct plane-wave solutions in frequency ω and wave vector $\theta \in \mathbb{R}^d$. Defining the wave-vector-dependent matrix function $\mathbb{A}(\theta) = \sum_{|\beta| \leq R} e^{-i\theta \cdot \alpha} A_\beta$, the computation of plane waves reduces to finding the branches $\omega = \Omega_j(\theta)$ of the dispersion relations $0 = \det(\omega^2 M - \mathbb{A}(\theta))$.

Various scalings

The transition from discrete lattice models to their continuum description on a macroscopic scale and to thermodynamics, whose structure will be described later on, can be established by a scaling transformation. To this end, we introduce the scaling parameter $\varepsilon = 1/N$, which is assumed to be small. Three steps are now necessary to reach the macroscopic scale. At first, we define macroscopic time, particle index, and space by

$$\tau = \varepsilon^\beta t, \quad y = \varepsilon^\gamma (\alpha - c_{\text{gr}} t), \quad \zeta = \varepsilon^\delta x, \quad (4)$$

where c_{gr} is the group velocity.

The constants β , γ , and δ indicate that various scalings are possible, which are fixed by a special choice of the values of these constants. In the second step, we introduce a two-scale ansatz for

the microscopic dynamics that embodies the expected physical phenomena on the macroscopic scale. In a third step, this ansatz will be inserted in the microscopic evolution equation, and there are already many examples where the leading order terms in ε represent the evolution on the macroscopic scale. For an illustration we will next consider several examples (see also [1], [2]).

Hyperbolic scaling and cold motion. We consider the atomic chain and choose $\beta = \gamma = \delta = 1$. In this case the simplest two-scale ansatz is introduced by

$$x_\alpha(t) = \frac{1}{\varepsilon} X(\varepsilon t, \varepsilon \alpha). \quad (5)$$

We insert this ansatz in the equations of motion (1) and obtain as leading order terms the PDE system

$$\partial_\tau r - \partial_y v = 0, \quad \partial_\tau v - \partial_y \Phi'(r) = 0, \quad (6)$$

with pressure $p = -\Phi'(r)$ and the definitions $r = \partial_y X$ and $v = \partial_\tau X$. This is the so-called nonlinear p -system, which is hyperbolic for $\Phi'' > 0$. Note that the two-scale ansatz (5) assumes that the microscopic motions of neighboring atoms do not differ very much. In other words, the ansatz does not allow for rapid oscillations, and thus we speak of *cold motion*, because only such oscillations could be called *temperature* on the macroscopic scale.

KORTEWEG–DE VRIES scaling. Our next example also concerns cold motion, but now we consider a different scaling, viz.

$$x_\alpha(t) = \varepsilon X(\varepsilon^3 t, \varepsilon(\alpha - ct)). \quad (7)$$

The macroscopic coordinates are thus given with respect to a frame that moves with c . In this frame higher order terms of NEWTON's equation vanish identically up to order 3, and the fourth order yields for $r = \partial_y X$ the KORTEWEG–DE VRIES equation

$$\partial_\tau r + r \partial_y r + \partial_{yyy} r = 0. \quad (8)$$

Note that the multiscale ansatz (7) implies on the macro scale the evolution of a pulse with small amplitude for very large times.

The dispersive scaling for the nonlinear SCHRÖDINGER equation. We consider now solutions of the general systems (2) having a simple microscopic structure that is modulated on much larger spatial and temporal scales. Assuming that (3) provides the linearization at $x_\alpha \equiv 0$, we choose a wave vector θ , a branch $\omega = \Omega_j(\theta)$ of the dispersion relation, and the associated eigenvector $\Phi_j(\theta)$. The corresponding group velocity is given by $c_{\text{gr}} = \nabla_\theta \Omega_j(\theta)$. With this knowledge from the linear theory we are interested in the macroscopic evolution of a modulated plane wave solution in the form

$$x_\alpha(t) = \varepsilon A(\tau, y) e^{i(\omega t + \theta \alpha)} \Phi_j + \text{c.c.} + O(\varepsilon^2), \quad (9)$$

with $\tau = \varepsilon^2 t$ and $y = \varepsilon(\alpha - c_{\text{gr}} t)$. Here, $A(\tau, y) \in \mathbb{C}$ is the macroscopic amplitude of the wave.

Since the system is dispersive and nonlinear, and the amplitude A is weakly scaled by $0 < \varepsilon \ll 1$, we need a slow macroscopic time scale $\tau = \varepsilon^2 t$ comparing to the macroscopic space scale $y = \varepsilon(\alpha - c_{\text{gr}} t)$, in order to see the evolution of A as time passes. This is the so-called *dispersive scaling*. The choice of y also reflects the fact that the macroscopic envelope A is moving with the group velocity c_{gr} , whereas the microscopic waves have the phase velocity $-\theta/\omega$.

Using formal expansion techniques, it turns out that the evolution of A must be governed by the nonlinear SCHRÖDINGER equation

$$i\partial_\tau A = \text{div}_y \left(\frac{1}{2} D_\theta^2 \Omega(\theta) \nabla_y A \right) + \rho |A|^2 A. \quad (10)$$

This formal derivation is justified in a series of papers, see [3]. It is shown there that solutions of (2) satisfying the ansatz (9) at $t = 0$ will keep this microscopic and macroscopic structure and are well described by the solutions of the macroscopic nonlinear SCHRÖDINGER equation on the corresponding long time intervals $[0, \tau_*/\varepsilon^2]$.

Three-wave interaction. Using the hyperbolic scaling, it is possible to observe the interaction of several pulses that are formed of different basic plane waves $e^{i(\omega_n t + \theta_n \cdot \alpha)} \Phi_n$. The simplest case occurs for the interaction of three waves, where the following resonance conditions are assumed to hold:

$$\theta_1 + \theta_2 + \theta_3 = 0 \pmod{\mathcal{T}} \quad \text{and} \quad \omega_1 + \omega_2 + \omega_3 = 0. \quad (11)$$

The solutions of (2) have the form

$$x_\alpha(t) = \varepsilon \sum_{n=1}^3 A_n(\tau, y) e^{i(\omega_n t + \theta_n \cdot \alpha)} \Phi_n + \text{c.c.} + O(\varepsilon^2),$$

with $\tau = \varepsilon t$ and $y = \varepsilon \alpha$. The amplitudes A_n , $n = 1, 2, 3$, satisfy the so-called *three-wave interaction equations*

$$\begin{aligned} \omega_1 \partial_\tau A_1 &= \omega_1 \nabla_\theta \Omega(\theta_1) \cdot \nabla_y A_1 + c \bar{A}_2 \bar{A}_3, \\ \omega_2 \partial_\tau A_2 &= \omega_2 \nabla_\theta \Omega(\theta_2) \cdot \nabla_y A_2 + c \bar{A}_1 \bar{A}_3, \\ \omega_3 \partial_\tau A_3 &= \omega_3 \nabla_\theta \Omega(\theta_3) \cdot \nabla_y A_3 + c \bar{A}_1 \bar{A}_2, \end{aligned} \quad (12)$$

where $c \in \mathbb{C}$ is an interaction constant that can be determined from the potentials V_β . Each equation consists of a transport part via the group velocity and a nonlinear coupling to the two other modes. Figure 2 illustrates the behavior. Without the resonance condition (11) being fulfilled, nonlinear terms would not arise and the pulses would just pass through each other.

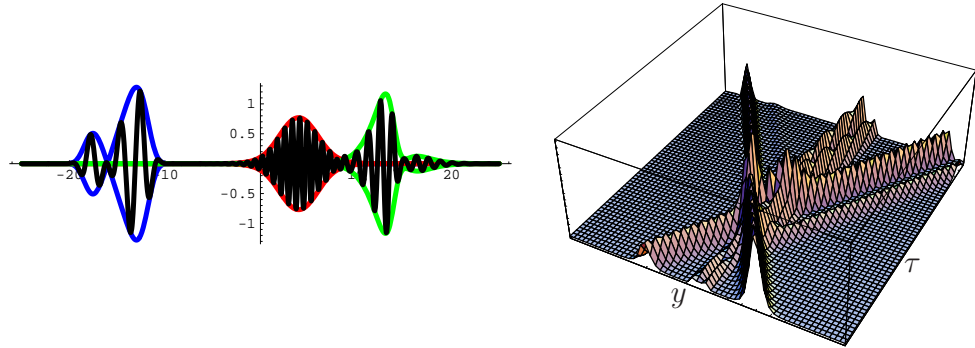


Fig. 2: Left: initial condition. Right: energy distribution in space-time

The three-wave interaction is used in data communication for transforming incoming signals A_1 with the carrier wave vector θ_1 into an outgoing signal A_2 with carrier wave vector θ_2 . Superimposing the incoming signal A_1 with a standard signal A_3 with wave vector θ_3 generates the desired signal A_2 via the nonlinearity $c \overline{A_1 A_3}$.

Hyperbolic scaling with temperature. Our last case concerns microscopic oscillations that are capable of generating temperature on the macroscopic scale. For this purpose, we introduce periodic traveling waves with four parameters. If these are constant, we find exact solutions to NEWTON's equation of motion. However, we are interested whether approximate solutions exist if the four parameters are modulated on the macroscopic scale so that they become functions of macroscopic time and space. In this case, the traveling wave parameters become the variables of the thermodynamic state of the microscopic structure. We expect that their evolution may be described by a system of four PDEs. Here, we start from the two-scale ansatz

$$x_\alpha(t) = \frac{1}{\varepsilon} X(\varepsilon t, \varepsilon \alpha) + \Upsilon(\varepsilon t, \varepsilon \alpha, \frac{1}{\varepsilon} \phi(\varepsilon t, \varepsilon \alpha)). \quad (13)$$

We call Υ the profile function, ϕ denotes the phase, and the macroscopic variables are defined by $r = \partial_y X$, $v = \partial_\tau X$, $\omega = \partial_\tau \phi$, $\theta = \partial_y \phi$ and denote macroscopic distance, velocity, frequency, and wave number, respectively. WHITHAM gives formal techniques, applicable to the LAGRANGIAN version of NEWTON's equation, to find the corresponding PDE system for these variables, which reads

$$\partial_\tau r - \partial_y v = 0, \quad \partial_\tau v + \partial_y p = 0, \quad \partial_\tau \theta - \partial_y \omega = 0, \quad \partial_\tau S + \partial_y g = 0. \quad (14)$$

The newly introduced quantities S and g may be interpreted as entropy density and entropy flux. We could show that the PDE system is closed by the so-called *internal energy of the traveling wave*

$$U(r, \theta, S) = \int_0^1 \left(\frac{1}{2} \left(\frac{\partial \Upsilon(\cdot, \phi)}{\partial \phi} \right)^2 + \Phi(r + \Upsilon(\phi + \frac{\theta}{2}) - \Upsilon(\phi - \frac{\theta}{2})) \right) d\phi, \quad (15)$$

which satisfies the GIBBS equations for the traveling wave $U(r, \theta, S)$,

$$dU = \omega dS - p dr - g d\theta. \quad (16)$$

The system (14) with (15) and (16) implies a further conservation law for the energy $E = K + U$, viz. $\partial_\tau E + \partial_y(q + pv) = 0$, where K , U , and q denote kinetic energy, internal energy, and heat flux. At least for the TODA interaction potential, we have a strict hyperbolic system.

A piece of thermodynamics

After these examples of various scalings, which lead to different classes of PDE systems, we illustrate some pieces of the structure of thermodynamics. This provides the general setting for those PDE systems that are in accordance with the physical laws and, in particular, with the *2nd law of thermodynamics*. Thermodynamics describes the evolution of deformation and heat in physical bodies on the macroscopic scale. Its strategy is as follows: In any space-time point (τ, y) of the body, a certain number of specific densities $u_j(\tau, y)$, $j = 1, \dots, M \ll N$, is declared as variables. For given initial and boundary data, these densities are determined by a system of PDEs that rely on balance equations, which read in regular points

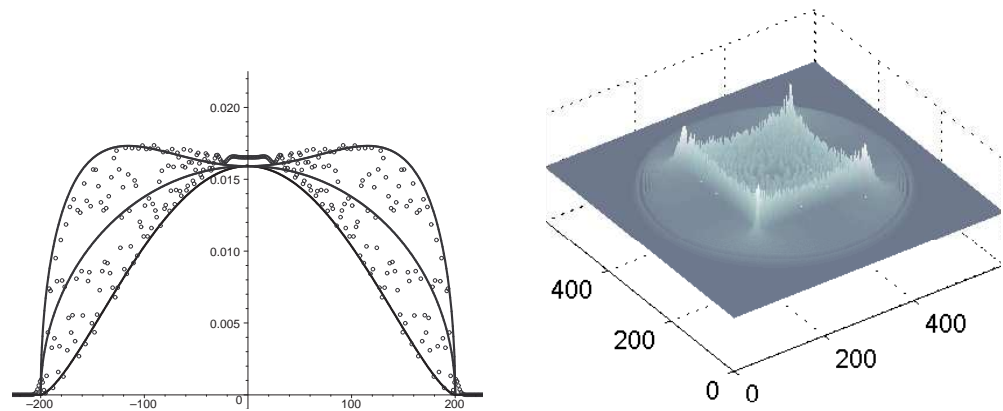
$$\partial_\tau u_j + \partial_y F_j = P_j, \quad j \in 1, 2, \dots, M, \quad (17)$$

where F_j and P_j are fluxes and productions, respectively. The most fundamental balance equations are the conservation laws, i.e., $P_j = 0$, for mass, momentum, and energy. In order to end up with a PDE system for the variables, the system of balance equations must be closed by constitutive laws for the fluxes and productions. These laws are restricted in their generality by the *2nd law of thermodynamics*, which implies the existence of a GIBBS equation and gives a definition of temperature, viz. $T = \partial U / \partial S$. We conclude that the traveling-wave ansatz leads to a macroscopic PDE system that fits into the framework of thermodynamics, because (i) it implies a GIBBS equation, (ii) it provides the identification $\omega = T$, and (iii) entropy flux and heat flux are related by $g = q/T$, which is important for the measurability of temperature.

Numerical examples

Energy transport in harmonic lattices. Even for the linear system (3), there are challenging questions concerning the convergence of the solutions to the PDE for linear elastodynamics. This relates to solutions without microstructure; however, solutions with microstructure behave differently as the energy is transported according to the group velocity associated with the dispersion relation. Using the WIGNER transform, which was originally developed in the context of the semiclassical limit in quantum mechanics, it was possible to show that this ballistic energy transport holds in the hyperbolic scaling $\tau = \varepsilon t$ and $y = \varepsilon x$. In Figure 3 we illustrate the distribution of energy in a linear system that was initially displaced only in one single atom.

Fig. 3: Left: energy distribution at $t = 200$ for the linear chain $\ddot{x}_j = x_{j+1} - 2x_j + x_{j-1}$ with initial data $x_j(0) = \delta_j$ and $\dot{x}_j(0) = 0$. Right: displacements for the square lattice \mathbb{Z}^2 with simple nearest-neighbor interaction at time $t = 120$



On the justification for the hyperbolic scaling with temperature. The mathematical justification of the PDE system (14) with (15) and (16) relies, in particular, on the problem whether solutions that start at time $t = 0$ as a traveling wave with modulated parameters will stay modulated traveling waves for macroscopically large time scales $t \in [0, \tau_0/\varepsilon]$ with $\tau_0 > 0$. Rigorous proofs are currently available only for the linear atomic chain and in the nonlinear case in the high temperature limit, see Figure 4 and [4], [5], [6].

Microscopic Dynamics for $N=64$

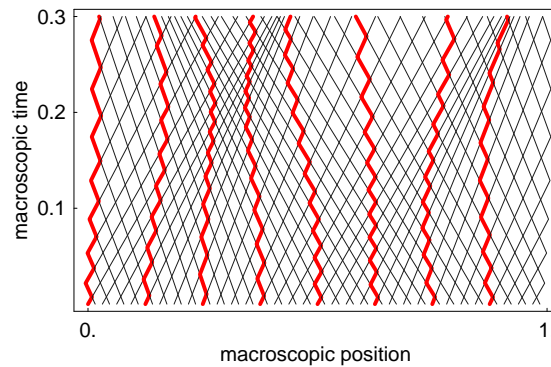


Fig. 4: Microscopic dynamics in the Euler picture for $N = 64$ particles in the high temperature limit, i.e., hard sphere collisions. The trajectories of some selected particles are indicated by red color.

On the other hand, numerical justification suggests the following behavior: 1. If all macroscopic fields are smooth, then the atomic data can be described in terms of modulated traveling waves whose parameters evolve on the macroscopic scale according to (14), (15), and (16). 2. Even shock-like structures that result from cold initial data can be described by modulated traveling waves; see Figure 5.

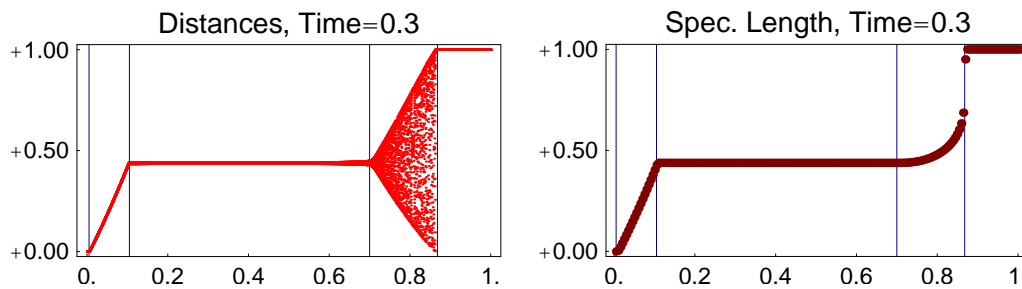


Fig. 5: Riemann problem with cold initial data $r_a(0) = 0$ for $y \leq 0.5$, $r_a(0) = 1$ for $y > 0.5$, $v_a = 0$ for $N = 16,000$ particles. Left: left-going wave remains cold, right-going wave develops temperature, i.e., rapid oscillations. Right: corresponding mean distances

3. If shocks are generated by data with temperature, traveling waves with a single phase variable fail to give the correct macroscopic limit.

Finally we mention a numerical experiment that seems to indicate that a parabolic scaling, i.e., $\beta = 2$, $\gamma = \delta = 1$, $c = 0$, might lead to a heat conduction equation. However, up to now the corresponding scaling limit could not be found. The initial data are as follows: Two half-chains L and R with MAXWELLIAN distributions with $T_L, r_L, v_L = 0$ and $T_R, r_R, v_R = 0$ of the atomic motion are brought in contact in order to start a RIEMANN initial value problem. Temperatures and distances are adjusted in a manner that leads to a continuous pressure so that waves are depleted. The resulting temperature field, see Figure 6, is obtained on the basis of 10^5 atoms, which is apparently not sufficient to reach the macroscopic limit. But even now we observe parabola-like structures indicating that $\xi^2/t = \text{constant}$, which is the proper behavior of the RIEMANN initial value problem for the heat equation.

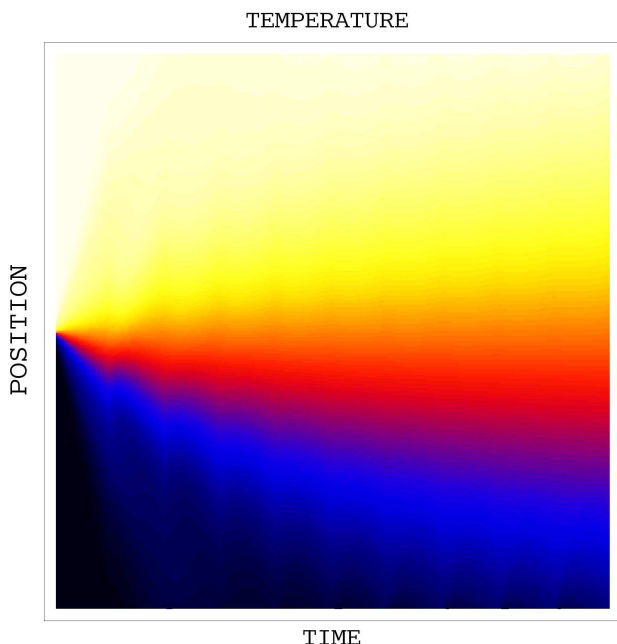


Fig. 6: Space-time representation of a temperature field in the atomic chain

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2.2 Optimization Problems with Random Constraints

René Henrion

Many optimization problems arising in engineering or manufacturing processes contain uncertain data that can be modeled by means of random variables. Typical examples are uncertain loads in electricity, water, or gas networks, uncertain meteorological conditions (e.g., precipitation in water reservoir management), uncertain costs (e.g., fuel), or uncertain geometric positions of objects (e.g., robotics). Thus, one is led to consider the following optimization problem subject to a random parameter:

$$\min \{f(x) \mid g(x, \xi) \leq 0\}.$$

Here, x and ξ denote random and decision vectors, respectively, f is an objective function to be minimized (e.g., costs), and g is a mapping describing technological constraints of the system under investigation. As g may have several components, the inequality sign is to be understood componentwise.

In many applications one is faced with so-called *here-and-now decisions*. This means that an optimal decision x has to be found prior to the observation of ξ . For instance, the design of technical constructions has to be determined in such a way that it resists future uncertain perturbations of some nominal load parameters. Then it does not make sense to solve the problem formulated above, because no specific value for ξ is available. Rather, one has to fall back on deterministic reformulations of this problem that cancel out its dependence on concrete realizations of ξ but take into account information on its distribution, possibly gathered from historical observations. Among others, the following model, called *probabilistic constraint*, is well introduced and widely applied in engineering:

$$\mathbb{P}(g(x, \xi) \leq 0) \geq p.$$

Here, \mathbb{P} denotes a given probability measure. In this model, a decision x is declared to be feasible if the inequality system $g(x, \xi) \leq 0$ is satisfied with a probability of at least p for some safety level $p \in [0, 1]$. The advantage of this last approach is that it offers decisions that are reasonably robust and at the same time not too expensive.

Figure 1 provides an illustration in the context of an obstacle problem: A manoeuvrable body (colored blue) has to be moved with its lower left corner from A to B along a shortest possible path, thereby avoiding collision with some obstacle. For simplicity, no angular movement is considered. The obstacle is assumed to be random in the sense that the position of its lower left corner follows a two-dimensional normal distribution. The figure shows ten simulated realizations of the obstacle (black) along with its expected value (red). The manoeuvrable body could represent the grip arm of a robot whereas the obstacle might be some workpiece repeatedly set down with a small inaccuracy. We want to find a robust, collision avoiding shortest path without knowing future positions of the obstacle. The thin curve joining A and B in the figure relates to the shortest path under the assumption that the obstacle takes its expected position. Looking at the simulated positions, it is clear that such a solution will end up in many future collisions (around 50% of the cases). In

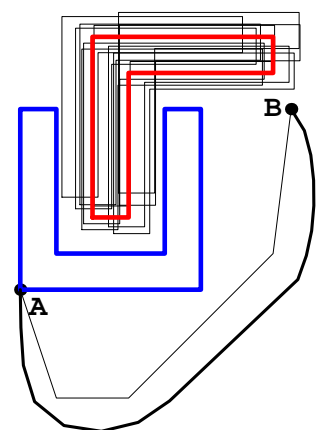


Fig. 1: A shortest path problem with a random obstacle

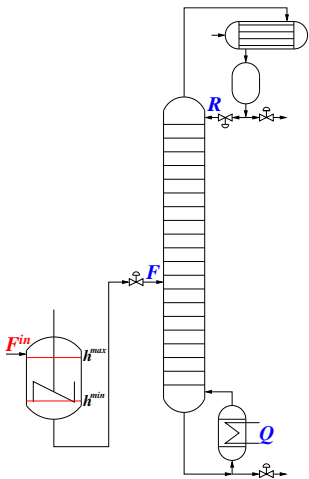


Fig. 2: Distillation column with feed tank

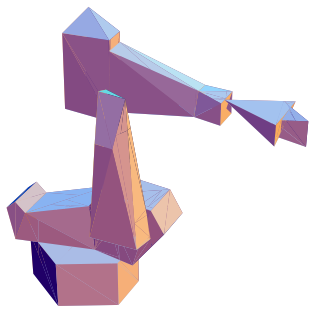


Fig. 3: Polyhedral approximation of a robot

contrast, the thick curve provides a shortest path under the probabilistic constraint of collision avoidance at probability $p = 0.8$. This provides a much more robust solution coming at the price of a slightly longer path. Note that this path cannot be obtained by simply avoiding the silhouette of a confidence region into which 80% of the obstacles realizations would fall. The latter approach is related to so-called *robust optimization* and generally yields much more expensive solutions (i.e., longer paths).

In practical applications, one frequently deals with linear probabilistic constraints, where the mapping g happens to be linear in the random parameter ξ . According to whether decision vector and random parameter appear separately or multiplicatively coupled, one has to distinguish the following two basic types of linear probabilistic constraints:

$$\mathbb{P}(L\xi \leq h(x)) \geq p, \quad (1)$$

$$\mathbb{P}(\Xi h(x) \leq b) \geq p. \quad (2)$$

In (2), the random parameter is given by a stochastic matrix. This type is relevant for so-called *mixture problems* as they arise in engineering (mixture of raw materials under lower or upper limits for positive or negative contaminations of certain ingredients) and finance (portfolio problems).

Also the separated type (1) has abundant applications in engineering, some of which are the object of research at WIAS. For instance, this type was used to model the robust control of a continuous distillation process with random inflow rate; see [1]. Here, the inflow is collected in a feed tank before it is directed to the distillation column in a controlled manner. For technological reasons, the filling level in the feed tank has to satisfy certain upper and lower limits (red lines in Figure 2). The feed extraction rate F was found in a way to keep the filling level at high probability between these levels and to operate the column at minimum heat consumption Q .

Another instance of type (1) arises in the modeling of collision avoidance between polyhedral controllable objects and polyhedral random obstacles, as it was sketched in a simplified setting in Figure 1. The assumption of polyhedrality guarantees that the probabilistic constraint becomes linear, which is important for its numerical solution. On the other hand, real-life objects from manufacturing processes, like workpieces or robots, can be approximated to any desired degree of precision by finite unions of polyhedra; see Figure 3, for an example of a rough approximation of a robot (data: I. Bremer, WIAS).

For yet another application of (1), we refer to capacity optimization in stochastic networks; see [6]. Figure 4 shows a simple example of a network the nodes of which represent random demands (black) or generating facilities (red) of a certain product (electricity, water, gas, etc.), whereas its arcs relate to transmission links between distinguished nodes. The generating and transmission capacities of the network have to be designed in such a way that random demands observed later on are met with high probability and that the overall costs are minimized. The left diagram of Figure 4 illustrates an optimal solution for a certain constellation under a probabilistic constraint with safety level $p = 0.9$. The magnitude of (expected) demands and generating capacities are

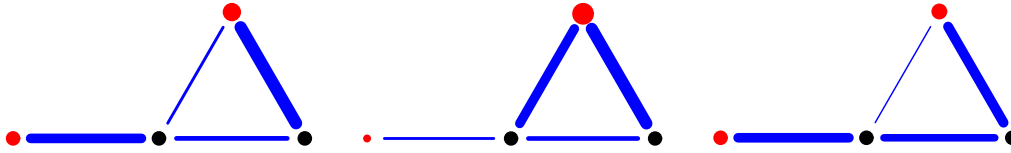


Fig. 4: Capacity optimization for a network with random demands

represented by disks of corresponding area, while transmission capacities are represented by the thickness of the lines. In this problem (and many others of similar type), one is faced with the existence of multiple solutions. The diagram in the middle of Figure 4 provides a different solution realizing the same costs and the same safety level. The right diagram of Figure 4 illustrates the effect of changing the distribution by passing from zero correlation in the first two diagrams to negatively correlated random demands. Here, the capacity of the transmission link between the nodes with random demands has increased.

Although probabilistic constraints induce a set of feasible decisions

$$M = \{x | \alpha(x) \geq p\}, \quad \alpha(x) := \mathbb{P}(g(x, \xi) \leq 0),$$

of seemingly conventional type, it has to be taken into account that the probability function α is not given by an explicit formula. The determination of its values and its gradients (if possible) represents the main challenge in the numerical solution of such problems.

Since a good theoretical understanding of probabilistic constraints is essential for the design of efficient algorithms, part of our work has focused on the analysis of structural and analytical properties of M and α , like convexity, compactness, continuity, or differentiability. These properties are not evident and cannot, in general, be recovered from the corresponding properties of the mapping g or the distribution of ξ . The first two diagrams of Figure 5 illustrate this fact for ξ having a one-dimensional normal distribution and $g : \mathbb{R}^2 \times \mathbb{R} \rightarrow \mathbb{R}^2$ representing two different affine linear mappings. Despite the fact that all input data of the probabilistic constraint look nice at first glance, the figure shows that α may happen to be nonsmooth or even discontinuous.

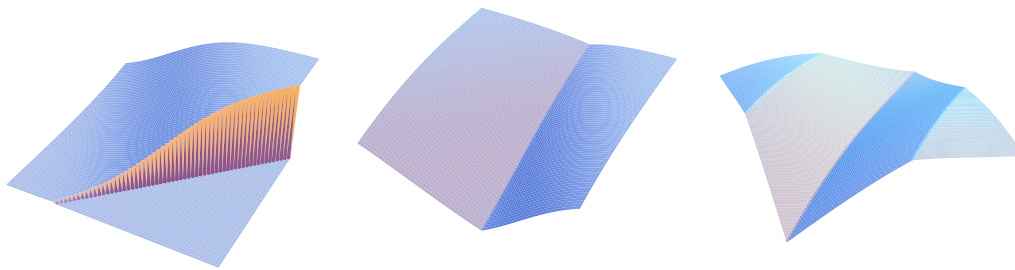


Fig. 5: Graphs of the probability function related to (1)

In [3], continuity and differentiability of the probability function associated with (1) have been investigated for ξ having a quasi-concave distribution. We recall that this class contains a large variety of prominent multivariate distributions (e.g., regular and singular normal, multivariate gamma, Dirichlet, uniform on compact convex sets, Pareto, etc.; see [6]). An equivalent characterization for continuity and Lipschitz continuity simultaneously was provided in [3]. It turns out that in case of the capacity expansion problem, α can be expected to be of class $\mathcal{C}^{1,1}$ if the distribution function

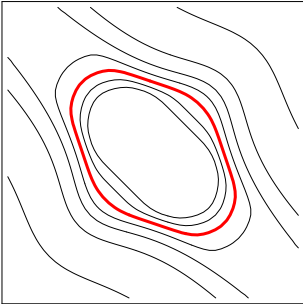


Fig. 6: Set of feasible decisions for different safety levels p

of ζ is smooth. In contrast to this, α is just Lipschitz continuous in the problem of collision avoidance, so one is inevitably led to a nonsmooth optimization problem here. A typical cross section of this function is shown in the right diagram of Figure 5.

One of the most interesting structural properties in optimization is the convexity of the set M of feasible decisions. For type (1), this question is satisfactorily answered by classical results due to Prékopa in case that all components h_i of h in (1) are concave [6]. Then, log-concavity of the multivariate distribution of ζ is sufficient to guarantee the convexity of M for all levels p . Beyond the case that the h_i are concave, this result does no longer hold true. Figure 6 illustrates an example where ζ has a bivariate normal distribution with independent components — which is log-concave — but with h_1, h_2 being strictly convex rather than concave. As one can see, M is nonconvex for some levels p , but it is eventually convex, i.e., convex for $p > p^*$ ($p^* \approx 0.7$ in the example; see red curve). Note that eventual convexity remains a practically useful property because the safety level is typically chosen close to one. In [4], it is shown how to explicitly calculate such critical level for ζ having independent components. The result applies basically to all classical (continuous) distributions and to mappings h whose components are r -concave for some $r < 0$.

Not too much is known about the convexity of the feasible set defined by (2), even in case of normally distributed Ξ and $h(x) = x$. Apart from the classical result by Van de Panne/Popp/Katoka, stating convexity for $p \geq 0.5$ if Ξ reduces to a single row, some generalizations can be found in [6], where special structures of the overall covariance matrix are assumed. It is interesting to observe that the analysis discussed before and designed for type (1) can be partially used for this second structure, too. Assuming that the rows ζ_i of Ξ are independently normally distributed with mean vectors μ_i and covariance matrices Σ_i , it was shown in [4] that the feasible set is eventually convex with

$$p^* = \Phi \left(\max \left\{ \sqrt{3}, u^* \right\} \right), \quad u^* = \max_{i=1, \dots, m} 4\lambda_{\max}^{(i)} \left[\lambda_{\min}^{(i)} \right]^{-3/2} \|\mu_i\|,$$

where Φ is the one-dimensional standard normal distribution function, and $\lambda_{\max}^{(i)}$ and $\lambda_{\min}^{(i)}$ refer to the largest and smallest eigenvalues of Σ_i .

Another important information on feasible sets in optimization is compactness. With the notation used before, compactness can be guaranteed for levels $p > p_1$, where

$$p_1 := \max_i \Phi \left(\sqrt{\langle \mu_i, \Sigma_i^{-1} \mu_i \rangle} \right).$$

It is important that these results not just formally state the existence of some critical level beyond which convexity or compactness holds true, but that it is actually possible to calculate this level explicitly from the distribution data.

When solving an optimization problem under probabilistic constraints, one has, in general, no or at most partial information about the distribution of the random vector. One might rather be able to estimate this distribution from historical observations and then calculate a solution of the problem based on this estimation. This immediately raises the question of solution stability under perturbations of the underlying probability distribution. Usually, with estimation based on a sample of size

N one associates the idea that the calculated solution will be close to the (or a) true one, whenever N is large enough. This does not have to be true, in general. Figure 7 shows the solution of a two-dimensional problem for an unstable probabilistic constraint under empirical approximation with sample size N . It can be seen that for $N \rightarrow \infty$ three different solutions can be obtained, whereas only one of them corresponds to the unique solution of the original problem (red circle).

In the stability analysis one has to take into account that there might exist multiple solutions to the original and the approximating problems (see remarks on the capacity expansion problem above). Therefore, one has to consider set-valued solution mappings with probability measures as parameters. It was shown in [2] that for convex objective functions and under a Slater-type condition, the solution set mapping behaves upper semicontinuous in the sense of Berge at log-concave probability measures. The optimal value function even turns out to be calm there, i.e., Lipschitz continuous with the first argument held fixed at the original measure. For convex-quadratic objective functions, the following much more powerful statement can be made on local Hausdorff–Hölder continuity at an original probability measure μ which happens to be even strongly log-concave:

$$d_H(S(\mu), S(\nu)) \leq L\sqrt{d_K(\mu, \nu)} \quad \forall \nu : d_K(\mu, \nu) < \delta.$$

Here, the term on the left-hand side denotes the Hausdorff distance between the solution set $S(\mu)$ of the original problem and the solution set $S(\nu)$ based on the approximating measure ν . On the right-hand side, d_K refers to the Kolmogorov distance between probability measures. Specifying this estimation to empirical approximations ν_N , the following exponential bound can be derived:

$$\mathbb{P}(d_H(S(\mu), S(\nu_N)) \geq \varepsilon) \leq C [N\lambda]^{s-0.5} e^{-2N\lambda},$$

where $\lambda = \min\{\delta^2, (\varepsilon/L)^4\}$, and s is the dimension of the random vector.

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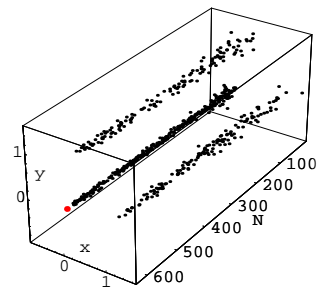


Fig. 7: Sample-based solution of an unstable problem with probabilistic constraints

2.3 Creating Novel Devices for High-speed Optical Telecommunications

Matthias Wolfrum, Mindaugas Radziunas, Uwe Bandelow, and Annegret Glitzky

Directly modulated lasers for high-speed signal conversion

In modern telecommunication systems, signals are electronically generated and then transmitted through optical fibers. Thus, devices for conversion of electronic signals into optical signals at high speed are key components in modern data communication networks.

Semiconductor lasers are able to realize this functionality just by modulating the pump current with the signal resulting in an intensity modulation of the emitted light. However, in conventional semiconductor lasers, the speed of this process is limited by about 10 GBit/s (10,000,000,000 Bits in one second). The reason for this limitation is that a semiconductor laser after a change in the pumping current typically shows an oscillatory relaxation to the new state of operation (see Figure 1). This is because the additionally supplied energy tends to fluctuate periodically between the carriers and the photons in the laser until the system relaxes to its new equilibrium state. As soon as the signal frequency reaches the time scale of this so-called *carrier-photon resonance*, the transmitted signal is spoiled by the oscillations.

In order to reach higher bit rates, more sophisticated devices with different dynamical properties are necessary. A large variety of dynamical features is known from multi-section lasers. These devices have a complex structure consisting of different sections where the light is modified in different ways. Combining active and passive sections, optical gratings or saturable absorption in a specific way, different devices for various purposes can be constructed. There exist multi-section lasers for the generation of short pulses, for synchronization to a pulsating signal, and even for synchronization to a chaotic signal.

But there was no concept of a multi-section laser for direct signal modulation at high speed, up to now. And even for the other existing device concepts, it is a challenging task to control, understand, and optimize the complex physical mechanisms leading to the specific dynamical behavior.

In this situation the engineers from the Heinrich Hertz Institute (HHI) of Fraunhofer Gesellschaft in Berlin came to WIAS with the question: Can one invent a multi-section laser with improved modulation properties? And, can this be done without numerous expensive and time consuming experiments, fabricating and measuring a lot of different possible laser configurations? At that time they had no idea for some mechanism or configuration in a multi-section laser that could supply the desired behavior. Instead, they came with a long list of possible candidates and the hope that under suitable operating conditions one of them could be able to do the job.

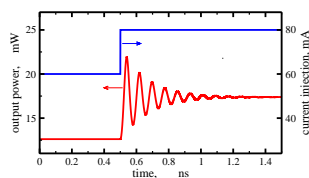


Fig. 1: Relaxation oscillations (red) due to carrier-photon resonance. Blue: injection current

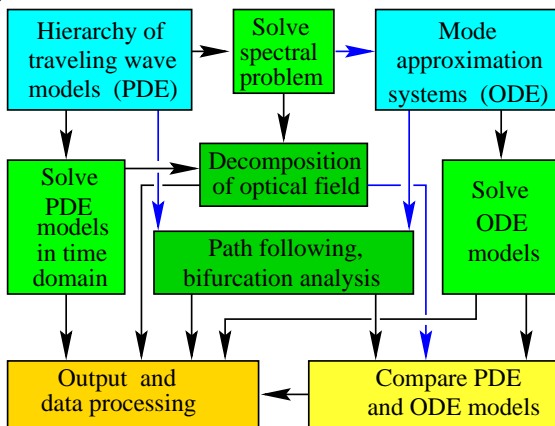
Exploring the dynamics of multi-section lasers with `LDSSL-tool`

Fig. 2: The software package `LDSSL-tool`

The reason why this question was addressed to WIAS was that the mathematical investigation of optoelectronic devices and, in particular, multi-section lasers was one of the main research topics at WIAS during the last years.

For the mathematical treatment of dynamical effects in multi-section lasers, WIAS researchers developed the software package `LDSSL-tool`. It has already been used for different types of multi-section lasers and contains algorithms for the simulation of the dynamical behavior of the devices, based on a nonlinear hyperbolic system of partial differential equations that describes the spatio-temporal evolution of the optical fields and the carrier inversion in the active semiconductor material.

Numerical simulation is like a virtual experiment: For a laser with specified design and operation conditions, the temporal evolution of the physical quantities describing the behavior of the laser can be computed. Additionally, the computed data can be automatically analyzed to detect the required device performance. In this way, `LDSSL-tool` allows to investigate a laser not only under different operating conditions like in a laboratory experiment, but also to change easily the design of the device, which in a real experiment would require an expensive and time consuming processing of a new device.

But `LDSSL-tool` can do even more. Based on so-called *path-following algorithms*, one can find directly the conditions that lead to a qualitative change in the dynamical behavior of the system. So-called *bifurcations* indicate how the dynamical behavior of the system depends on different control and design parameters. The application of numerical bifurcation analysis to the laser model by standard techniques is not directly possible, but requires a reduction to so-called *inertial manifolds* (see Figure 2), and is based on pioneering theoretical results about the applicability of this method to certain systems of hyperbolic partial differential equations [1].

Another expertise of WIAS lies in the field of simulating carrier transport in semiconductor devices by so-called *drift-diffusion models*. Using the software `WIAS-TeSCA` it is possible to simulate how a high-frequency electrical signal propagates in the complex transversal structure of the laser

until it finally reaches the optically active zone, where it interacts with the photons and contributes to the lasing process, which is modeled within `LDSL-tool`.

With the support of Investitionsbank Berlin (IBB), the Heinrich Hertz Institute initiated the project diMOLA to approach the problem of creating a multi-section laser for direct signal modulation supported by theoretical investigations at WIAS. In this project the possibilities for a new device concept should be first explored theoretically at WIAS, and then, if a design principle with suitable performance could be found, realized experimentally at HHI.

A new device concept, using photon-photon resonance and feedback stabilization

Now the exploration began: With new routines for an automatic validation of the device performance, hundreds of different laser configurations were simulated with `LDSL-tool`. Parallely, `WIAS-TeSCA` was used to find an optimal transversal structure for the device and to obtain an understanding of the signal transmission into the active zone of the laser.

Soon there were some indications that a passive feedback laser could be a promising candidate: A device consisting of an active DFB (distributed-feedback) section and a passive feedback section for phase tuning showed under certain operation conditions improved modulation properties.

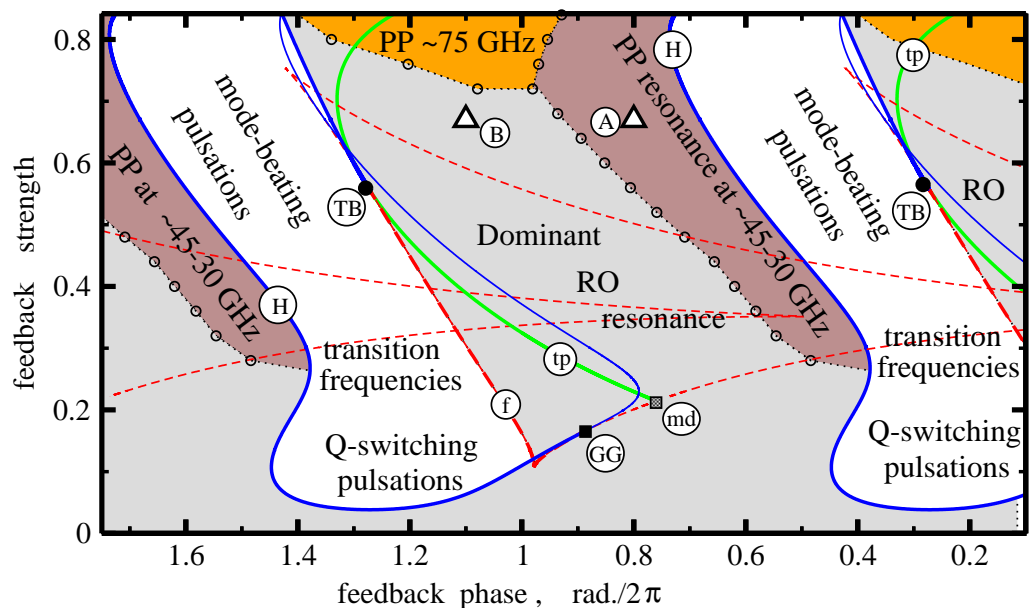


Fig. 3: Bifurcation diagram for passive feedback lasers

The goal was now to understand the physical mechanism behind this particular behavior in order to learn how this could be controlled and improved. The main control parameters for a feedback laser are the feedback strength and the feedback phase. For the design of the device, the length of the feedback section plays an important role, since the round-trip time of the light through this section determines the delay of the feedback signal.

Figure 3 shows a bifurcation diagram for a passive-feedback laser indicating the dynamical properties for all possible values of feedback strength and the feedback phase: In addition to several states of stationary lasing, there are different types of pulsations, but also complicated dynamics like homoclinic chaos, multi-stability, or so-called *Takens–Bogdanov points (TB)*. The improved modulation properties can be found near the point A in this figure. There, two particular things happen at the same time: The usual carrier-photon relaxation oscillation (RO) is suppressed and a new behavior called *photon-photon resonance (PP)* appears. In this dynamical process fluctuations happen between photons of two different optical frequencies. But since photons are much “smaller” and faster than electrons, these fluctuations have a much higher oscillation frequency and hence allow for much faster signal transmission.

In this way, it was possible to determine the optimal design and operation conditions for this effect. Figure 4 shows the theoretically predicted behavior of the optimized device under realistic operation conditions with 40 GBit/s random data signal. Panel (a) shows the injected signal (red) and the optical response (blue) of the laser. Sampling the output signal with the signal frequency, one obtains a so-called *eye diagram* (b). For an error-free data transmission, the eye has to be open, i.e., there should be a gap, allowing a clear distinction between a signal “0” and “1”. This is depicted in (c), where the signal distribution within the dashed rectangle in (b) is displayed.

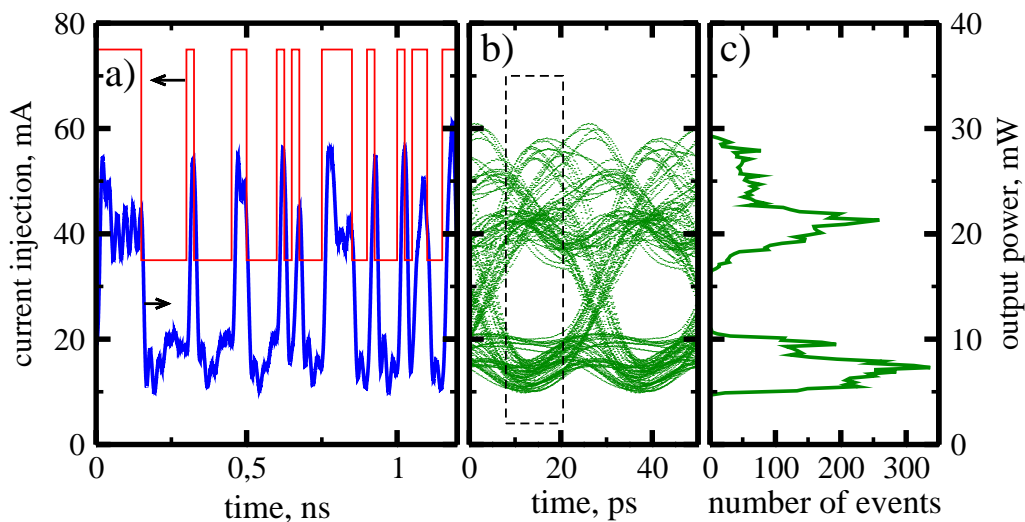


Fig. 4: Theoretically predicted signal transmission: (a) input and output, (b) eye diagram, (c) sampled distribution of signals “0” and “1”

The experimental realization

After this very promising theoretical outlook, everybody who was involved in the project was waiting eagerly for the first experimental results. Were all theoretical assumptions in the modeling really made correctly? Would the predicted effect really happen in this way? The experimental data readily exceeded all expectations. The quality of the transmitted signal was even better than in the simulations. The new device is now submitted for patent protection and will surely be part of future high-speed communication networks.

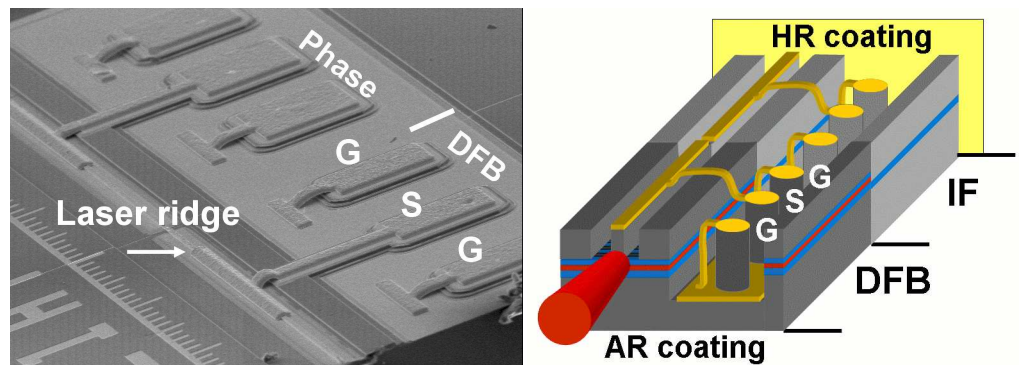
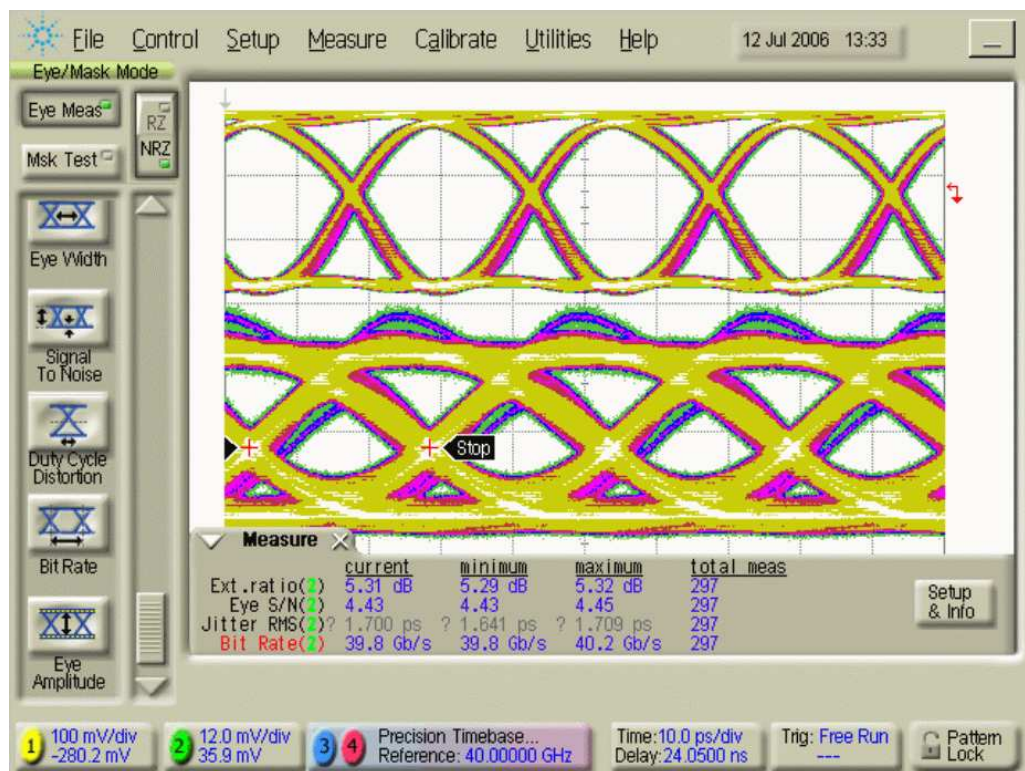


Fig. 5: The real device from Heinrich Hertz Institute and its performance: passive feedback laser and measured eye diagrams



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2.4 Three-dimensional Boundary Conforming Delaunay Mesh Generation — The TetGen Project

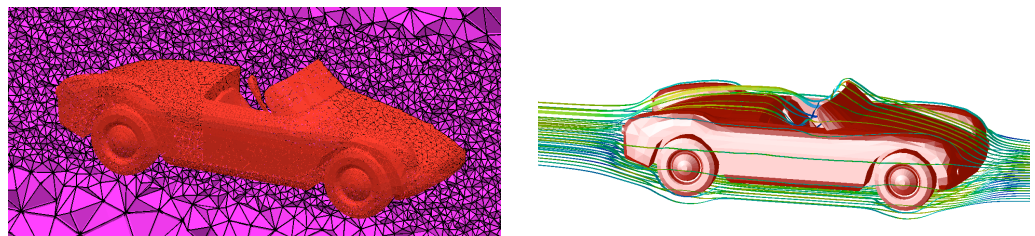
Hang Si, Jürgen Fuhrmann, and Klaus Gärtner

Background and motivation

Mesh generation is the process of partitioning a domain Ω into a set of simple geometric elements, such as triangles or quadrilaterals in two dimensions, or tetrahedra or hexahedra in three dimensions. It is used in a wide variety of fields: computer-aided design, geographic information systems, mathematical modeling, We are interested in the computer simulation of physical and engineering problems described by partial differential equations and use *finite element* and *finite volume* methods.

We assume that the domain Ω is the union of non-overlapping subdomains Ω_i , $i = 1, \dots, l$, $\Omega = \cup_i \Omega_i$. These subdomains can be used to model discontinuous material properties. The very first step in solving the problem numerically is to create a suitable mesh in Ω . This process has a tremendous effect on the computed results, either in the numerical error or in the computer resources used. Figure 1 shows a mesh of moderate complexity and the numerically computed velocity field.

Fig. 1: Left: a tetrahedral mesh around an automobile. Right: Stream lines visualize the computed velocity field.



Quality mesh generation. For different numerical problems, the focus is on different mesh properties. A classical numerical analysis result relates the interpolation error to the largest dihedral angle of an element. Small angles result in poorly conditioned stiffness matrices. Hence both large and small angles should be avoided in the final mesh. Problems requiring the fulfillment of L^∞ bounds are often treated by finite volume methods and can be solved on *boundary conforming Delaunay grids*. Internal or boundary layers in the solutions require anisotropic elements aligned to local orthogonal coordinates. These aspects can not be fulfilled equally well by a general-purpose grid generator, some of them can not be guaranteed for space dimensions larger than two. In other words: Many questions regarding grid generation in $N \geq 3$ dimensions are present and are future research topics. In [1] the reader will find an excellent overview and many references to classical results.

Delaunay meshes and Voronoi diagrams. Let E_i^N denote the simplex i with positive volume in N dimensions with vertices \mathbf{x}_i , $i = 1, \dots, N+1$. Each subdomain is represented by $\Omega_j = \cup_l E_l^N$. A Delaunay mesh of a point set is formed by simplices such that the ball defined by the $N+1$ vertices for all E_i^N does not contain any vertex $\mathbf{x}_k \in E_j^N$, $\mathbf{x}_k \notin E_i^N$.

The Voronoi volume of $V(\mathbf{x}_i)$ of a vertex \mathbf{x}_i is defined by $V_i = \{\mathbf{x} \in \mathbb{R}^N : \|\mathbf{x} - \mathbf{x}_i\| < \|\mathbf{x} - \mathbf{x}_j\|, \forall \text{ vertices } \mathbf{x}_j \in \Omega\}$. The corresponding Voronoi surface is given by $\partial V_i = \bar{V}_i \setminus V_i$.

A Voronoi diagram and the Delaunay mesh of a point set are dual in the following sense: The edges connecting the vertices in the Delaunay grid are orthogonal to the Voronoi surfaces.

Boundary conforming Delaunay meshes are Delaunay meshes with the property that all circumcenters of E_i^N are contained in $\bar{\Omega}_j$.

Boundary conforming Delaunay meshes just summarize all the properties to guarantee L^∞ bounds for reaction-convection-diffusion equations discretized by Voronoi-based *finite volume methods* [2]. That is one reason to be interested in boundary conforming Delaunay meshes from the numerical analysis point of view.

Algorithms to construct boundary conforming Delaunay meshes with guaranteed angle bounds are not known up to now. Only few algorithms can guarantee conforming Delaunay grids. They have either strong limitations regarding the input or are not practical, e.g., the computational time may be very large and the resulting mesh size can be unbounded.

Methodology

We now present our methodology. It treats the problem in two steps: boundary recovery and mesh refinement.

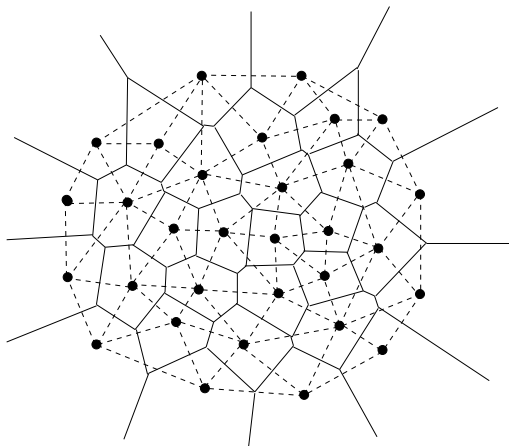


Fig. 2: The Voronoi diagram (solid lines) and its dual Delaunay triangulation (dashed lines) of a set of points in the plane.

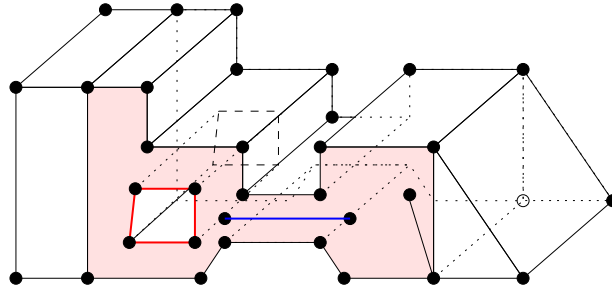


Fig. 3: Example of a piecewise linear complex (PLC). It shows a facet (shaded area) including a hole (red) and an isolated segment (blue).

Input geometry description of a domain. In order to describe the input geometry, we choose the boundary representation as a piecewise linear complex (PLC): A PLC X is a set of vertices $\mathcal{P} \subset \mathbb{R}^3$, segments \mathcal{S} , and planar facets \mathcal{F} . A facet $f \in \mathcal{F}$ may be of arbitrary polygonal shape, it may be non-convex, and it may contain holes. To be a complex, the components of X can only intersect at their common faces, which also belong to X . A PLC is not necessarily a manifold, it can contain internal facets and separated regions.

Three-dimensional boundary recovery. Given a PLC $X = (\mathcal{P}, \mathcal{S}, \mathcal{F})$, we want to find a tetrahedralization \mathcal{T} of \mathcal{P} such that \mathcal{T} respects all constraints (\mathcal{S} and \mathcal{F}) of X , and the number of tetrahedra in \mathcal{T} is minimal. It is known that even a simple non-convex polyhedron may not be tetrahedralizable without adding new points (called *Steiner points*). The problem of deciding whether a simple polyhedron can be tetrahedralized is NP-hard [3]. The problem of finding a minimal tetrahedralization is also known as NP-hard [4]. Nevertheless, we know that every polyhedron with n vertices can be tetrahedralized (with Steiner points) by $O(n^2)$ tetrahedra. This is known to be optimal in the worst case [4]. Of course, in many cases it is possible to do much better. In [5] we presented a method to decompose an arbitrary PLC into a *constrained Delaunay tetrahedralization* (CDT). A CDT is a well-suited structure for this problem. It has properties close to a Delaunay tetrahedralization, but it also respects the constraints. Our method successfully resolves the problem of non-existence of a CDT by constructing a suitable PLC, which is topologically and geometrically equivalent to the input PLC, and does have a CDT. This construction is performed by segment splitting and vertex perturbation. This method has been implemented in the mesh generator TetGen [7].

Adaptive constrained Delaunay refinement. A constrained Delaunay tetrahedralization (CDT) is generally not suitable for numerical computation. It may contain many badly-shaped tetrahedra. Furthermore, the size of tetrahedra may be too large. Hence both the quality and the mesh size of the CDT need to be improved in order to meet the basic requirements of numerical methods. This could be done by any mesh refinement method, but in general, the Delaunay property would be lost.

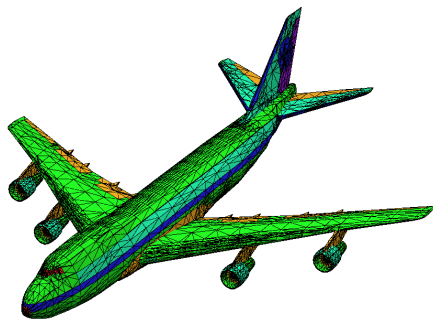
In paper [6], we developed a CDT refinement algorithm that uses the classical Delaunay refinement scheme. It generates an isotropic mesh corresponding to a sizing function, which can be provided by the user or is automatically derived from the input CDT. The tetrahedra of the produced mesh have a bounded circumradius-to-shortest-edge ratio. Slivers, tetrahedra formed by four nearly coplanar vertices, are found in the neighborhood of small input angles. Good mesh conformity

can be obtained for smoothly changing size information. The conforming Delaunay property is theoretically guaranteed in cases with input angles larger or equal 90° . In practice, the angle limit can be as small as 60° . This algorithm has been implemented in TetGen [7]. Up to complete sliver removal, the present status of TetGen fulfills the requirements of many finite element applications.

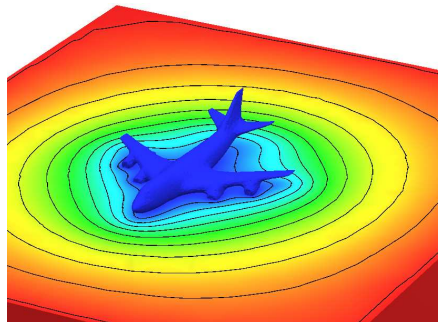
Examples

The following examples illustrate the interplay of the resulting grid and the size information for the tetrahedra provided by the user or derived from the input data.

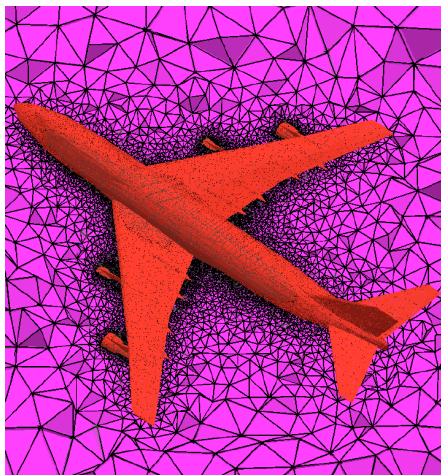
The first example is a Boeing 747 model in a bounding box. The input is a complicated surface mesh (2,874 nodes and 5,738 triangles). The tetrahedral mesh is constructed to compute a potential flow around the Boeing 747. The tetrahedra size information is explicitly given by a smoothed function of the Euclidian distance from the surface grid. The related grid providing this information has been generated by TetGen with low quality requirements.



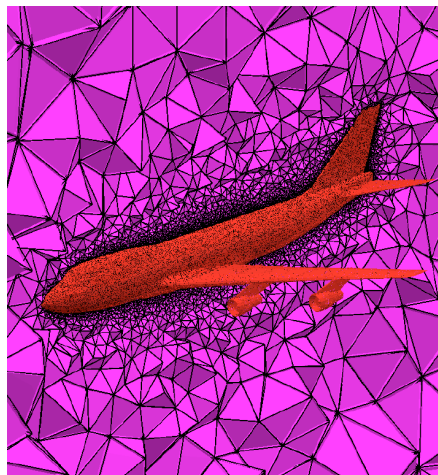
(a) The surface mesh



(b) Tetrahedra size information on a cut through the box, blue: small size tetrahedra, red: large size tetrahedra.



(c) Mesh detail (490,692 nodes and 2,709,770 tetrahedra)



(d) Mesh detail, refine time 59 s (44,500 tet/sec), 3.60 GHz Intel PC

Fig. 4: Adaptive tetrahedral mesh of the Boeing 747 model

The second example (Figure 5) illustrates the use of adaptivity and is part of the project `WIAS_Sharp` (see page 142). A moving laser spot heats a workpiece. Adaptive boundary conforming Delaunay meshes are generated whenever the estimated error in the solution gets larger than a user-specified accuracy. The grid gets coarse again in the already cooled-down regions, where the estimated error is small.

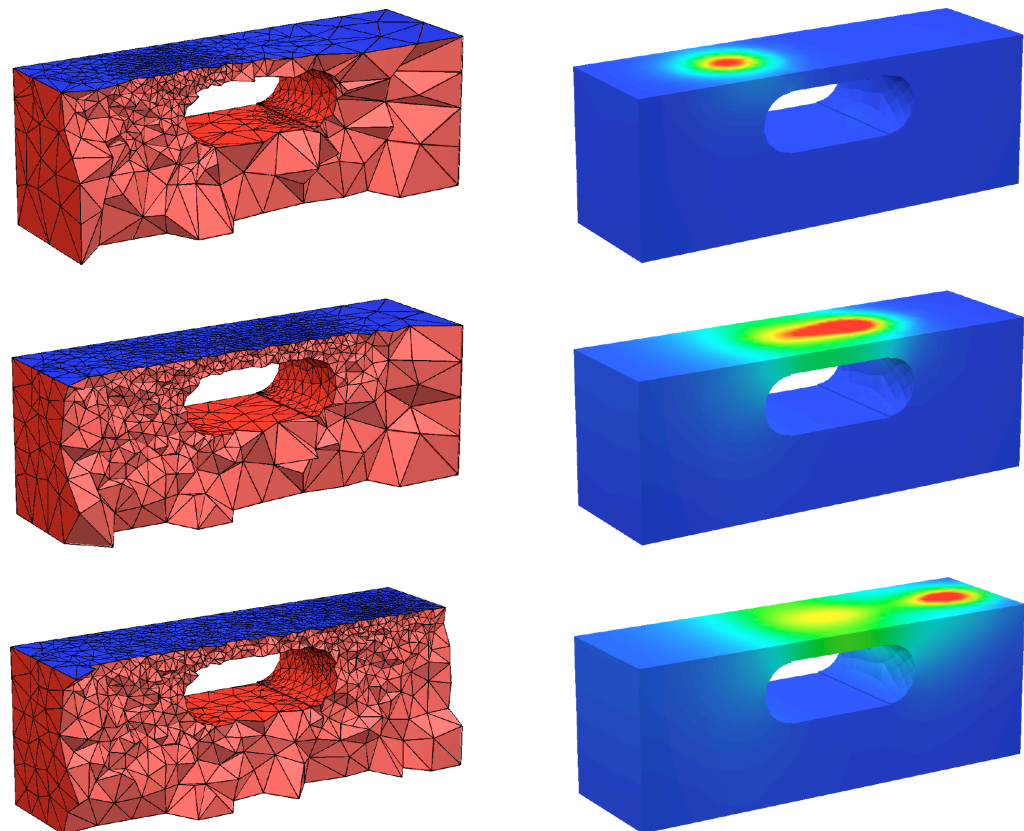


Fig. 5: A sequence of adaptive meshes related to the moving laser spot (left) and the temperature distributions (right)

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2.5 Applied Mathematical Finance: Iterating Cancelable Snowballs and Related Exotic Products

Christian Bender, Anastasia Kolodko, and John Schoenmakers

The scope of the project *Applied Mathematical Finance* is to provide new mathematical methods and efficient algorithms for the evaluation of financial instruments and the financial risk entailed in high-dimensional models. Problems arising in the financial industry, such as the evaluation of financial derivatives, generally involve the interplay of the *modeling of underlying financial data*, the *evaluation of financial products*, and *model calibration*.

In particular, effective valuation procedures for callable or cancelable high-dimensional financial products (also called *exotic options*) are considered a thorny problem. As a matter of fact, all standard industrial methods reveal limitations in the evaluation of these products. Christian Bender, Anastasia Kolodko, and John Schoenmakers ally these methods with their recent iterative improvement methodology developed at WIAS [2], [4], thus filling the final gap. In this article, an excerpt of [3], we give a sketch of their approach by exemplifying the valuation of a complex-structured cancelable product, the in the financial industry highly popular *cancelable snowball swap*.

Path-dependent cancelable products

A cancelable financial product is typically a contract that specifies a stream of cash payments or cash liabilities at fixed dates in the future. Generally, these future payments depend on the future state of underlying economical quantities, in our example interest rates, and are thus not known at the time the contract is signed. In the snowball, for instance, instead of paying the spot rate on a certain loan, the contract could prescribe to pay a fixed rate, plus yesterday's rate, minus today's spot rate, up to cancellation. Clearly, as soon as the spot rate falls too rapidly, the snowball will be canceled.

Mathematically more precisely, for a set of calling dates $0 < T_1 < \dots < T_k$, and cash flows C_i specified at T_i , we consider a contract that involves the right to cancel a stream of (possibly negative) cash flows C_1, \dots, C_τ , at a date τ to be decided by the holder of this contract. The cash flows of this product are equivalent to an aggregated cash flow $B_*(T_\tau)Z_\tau := B_*(T_\tau) \sum_{j=1}^{\tau} Z_j$ at the cancellation date, with $Z_i := C_i/B_*(T_i)$ being discounted cash flows with respect to some numeraire B_* (for example, a bank account). Indeed, it is equivalent to invest each cash flow C_i , $i \leq \tau$, in the numeraire B_* , yielding an amount $C_i/B_*(T_i) = Z_i$ that is worth $B_*(T_\tau)Z_i$ at date τ . By general arguments, the value of the cancelable product at time zero is given by

$$V_0^{cancel} := \sup_{\tau \in \{1, \dots, k\}} E^0 Z_\tau = \sup_{\tau \in \{1, \dots, k\}} E^0 \sum_{j=1}^{\tau} Z_j, \quad (1)$$

where the supremum is taken over all stopping rules with values in the set $\{1, \dots, k\}$ ($\tau = k$ may be interpreted as “not canceled”).

Iterating path-dependent cancelables

The path-dependent cancelable product introduced above can be seen as a standard (Bermudan) callable product with respect to a (virtual) cash flow Z_i . Therefore, it can be evaluated by an iterative method that has been developed in [2], [4].

Let us briefly recall this iterative method. Suppose we are given some (generally suboptimal) exercise policy τ_i , $i = 1, \dots, k$, for a Bermudan product with cash flow process Z ; τ_i is the stopping rule according to which the option should be exercised, provided the option has not been exercised before \mathcal{T}_i . This policy provides a lower bound process Y_i for the discounted Bermudan prices Y_i^* , also called *Snell envelope*,

$$Y_i^* \geq Y_i := E^i Z_{\tau_i}, \quad i = 1, \dots, k,$$

where E^i denotes the conditional expectation with respect to $\mathcal{F}_{\mathcal{T}_i}$. We next construct a new exercise policy ($0 \leq i \leq k$),

$$\hat{\tau}_i := \inf \left\{ j \geq i : Z_j \geq \max_{p: j \leq p \leq k} E^j Z_{\tau_p} \right\}, \quad (2)$$

and consider the new lower bound process,

$$\hat{Y}_i := E^i Z_{\hat{\tau}_i}, \quad i = 1, \dots, k,$$

which is generally an improvement of Y ,

$$Y_i \leq \hat{Y}_i \leq Y_i^*, \quad i = 1, \dots, k.$$

For a path-dependent cancelable product, the improved policy (2) reads ($0 \leq i \leq k$),

$$\hat{\tau}_i = \inf \left\{ j \geq i : 0 \geq \max_{p: j+1 \leq p \leq k} E^j \sum_{q=j+1}^{\tau_p} Z_q \right\}. \quad (3)$$

In most cases, both the cash flow Z_i and the event $\{\tau_i = i\}$ are determined by the state of an underlying Markovian process at date i . In such a situation, the conditional expectations involved in the iterative procedure can be estimated by Monte Carlo simulation, which leads to a Monte Carlo algorithm in a natural way.

In principle, we may iterate the above procedure, that is, improve $\hat{\tau}$ in the same way, and so forth. It is shown that after iterating this procedure $k - 1$ times, the Snell envelope is attained independently of the choice of the starting stopping family.

Generic construction of a good input stopping family

By choosing the trivial family $\tau_i \equiv i$, we are faced with the evaluation of the conditional expectations $E^j Z_q$ for $q > j$, hence European options, in (3). When these are available in closed form,

we may compute \widehat{Y}_i via (standard) Monte Carlo simulation and arrive at a next improved estimation $\widehat{\widehat{Y}}_i$ via a nested Monte Carlo simulation. However, closed-form Europeans are not known in all situations. For such cases, we will consider three kinds of input families, an Andersen-like (1999) method, Piterbarg's (2004) version of the Longstaff & Schwartz (2001) regression method, and a backward optimization of the exercise boundary resulting from the latter approach.

Andersen-like method: As a starting policy one could take

$$\tau_i^A := \inf\{j \geq i : H_j \geq Z_j\}, \quad (4)$$

where the deterministic sequence H is pre-computed via a standard optimization procedure as studied in [1] for Bermudan swaptions. The family $\widehat{\tau}$ obtained via (3) is then an improved exercise policy in the sense that $\widehat{\widehat{Y}}_i$, which requires nested Monte Carlo simulation, is generally closer to Y^* .

Longstaff & Schwartz à la Piterbarg: By the Longstaff & Schwartz (2001) algorithm, one may construct working backwardly an approximate continuation rest-value process of the form $C_j = C(j, L(\mathcal{T}_j))$. The functions $C(j, \cdot)$ are computed via a least-squares regression procedure, using a suitable system of base functions and a pre-simulation of the underlying process. After this, we next obtain a lower biased approximation of the Bermudan price by an independent Monte Carlo re-simulation and, using the stopping rule

$$\tau_i^{LS} = \inf\{j \geq i : C_j \leq 0\} \quad (5)$$

on the re-sampled trajectories.

For the typically high-dimensional (Libor) interest rate process, the choice of base functions in the regression procedure is often a problematic issue. To keep the regression method robust, Piterbarg (2004) suggests considering base functions that are only defined on a small set of explanatory variables, though he accepts *a priori* a bias in this way. As a generic choice, he proposes the short-term rate and the long-term rate. In our experiments, we will see that we may so obtain relatively close lower bounds for the cancelable snowball swap, but, particularly in more factor cases, these are not close enough.

Backward optimization of a given exercise boundary: As with the optimization procedure for (4), we may improve the exercise criterion obtained by the regression method to

$$\tau_i^{LS,A} = \inf\{j \geq i : C_j + \alpha_j \leq 0\}, \quad (6)$$

by backward optimization of the deterministic sequence α .

Our experiments show that the input stopping family (5) is generally insufficient in the sense that the gap due to the improved lower bound $\widehat{\tau}^{LS}$ and the dual upper bound corresponding to τ^{LS} is still too large. In all our cases, however, the gap due to $\widehat{\tau}^{LS,A}$ and the dual corresponding to $\tau^{LS,A}$ is acceptably small (though the lower bound due to $\tau^{LS,A}$ may be not sufficiently close). Therefore, we recommend (6) as a generically “good” input stopping family.

Specification and valuation of the cancelable snowball swap

Many cancelable structures in the financial industry are based on (future) interest rates. As such they involve the dynamics of the so-called *interest rate yield curve*, also called *Libor curve*. A Libor rate is usually a three- or six-month effective rate that is traded in the interbank market.

As an example, let us consider a snowball swap contract on a \$1 nominal loan. According to this contract, one receives floating Libor and has to pay so-called *snowball coupons* following the term sheet that one pays a constant rate I over the first year on a semi-annual basis, and in the forthcoming years $(\text{Previous Coupon} + A \cdot \text{Libor})^+$, where A is specified in the contract. A cancelable snowball swap is a snowball swap that may be canceled after the first year. The underlying interest rates are modeled by a (semi-annual) Libor model of forward Libors L_1, \dots, L_{n-1} , with $L_j(t)$ being the effective forward rate over period $[T_j, T_{j+1}]$ seen at time t , $0 \leq t \leq T_j$, $0 \leq j \leq n$, where $T_j := j \cdot 0.5$ are semi-annual forward tenor times.

As a case study, we consider a ten-year snowball contract with 19 semi-annual exercise possibilities starting at year one. In the contract, we take $I = 7\%$ and A increasing according to $A_2 = 3\%$, $A_{i+1} = A_i$, if i is even, and $A_{i+1} = A_i + 0.25\%$, if i is odd. For this example snowball, we present different methods for computing its value V_0 . To this end, we evaluate V_0 via a Monte Carlo algorithm for the iteration procedure (3) using different starting policies described above.

Numerical results: The underlying Libor rates were modeled using a standard *Libor Market Model*, which is calibrated to actual market data. For the stopping rules τ^A , τ^{LS} , and $\tau^{LS,A}$, we construct lower bounds, their corresponding dual upper bounds using the duality method developed in [7], and the improved lower bounds via (3), using different numbers d of driving random sources.

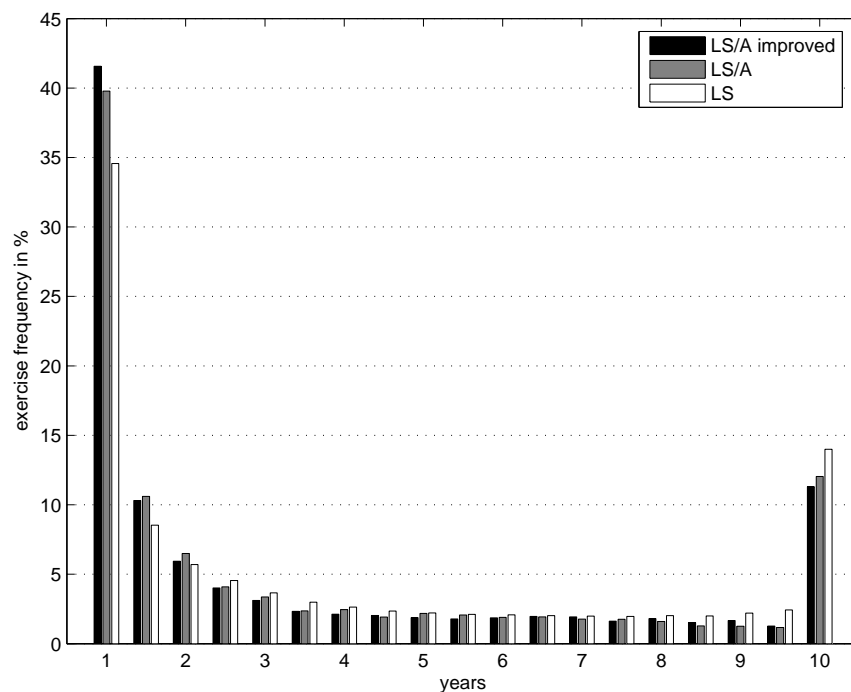
Figure 1 shows a typical picture of the exercise frequency of the cancelable snowball. It gives an impression of the high sensitivity of the product; the snowball swap is mostly canceled quite early or very late. It turned out that the price gaps due to improved Andersen's lower bound and Andersen's upper bound $(\hat{Y}_0^A, Y_{up,0}^A)$, respectively improved Longstaff–Schwartz and its upper bound $(\hat{Y}_0^{LS}, Y_{up,0}^{LS})$, were still unacceptable (up to 25%, 15% relative to prices, respectively). However, the price intervals $(\hat{Y}_0^{LS,A}, Y_{up,0}^{LS,A})$ could be considered tight enough. Indeed, from Table 1 we see that the gap is within 1% overall.

So we conclude with the following trust: *Iterate (once) the stopping strategy obtained via an Andersen-like enhanced Piterbarg version of Longstaff–Schwartz, and compute its dual due to Rogers, Haugh, and Kogan.*

d	$Y_0^{LS,A}$ (SD)	$\hat{Y}_0^{LS,A}$ (SD)	$Y_{up,0}^{LS,A}$ (SD)
1	215.00(0.40)	216.78(0.70)	218.12(0.42)
2	150.26(0.37)	156.79(0.74)	159.02(0.45)
5	111.62(0.35)	123.22(0.87)	126.63(0.51)
10	100.27(0.34)	112.97(0.86)	116.23(0.54)
19	93.52(0.34)	106.47(0.84)	110.22(0.55)

Table 1: Price estimations via $\tau^{LS,A}$

Fig. 1: Simulated exercise frequencies of τ^{LS} , $\tau^{LS,A}$, and $\hat{\tau}^{LS,A}$



Acknowledgment

The authors are grateful for interesting discussions with the Quantitative Analysis Department at Bankgesellschaft Berlin AG, on this subject.

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3 Research Groups' Essentials

- *Partial Differential Equations*
- *Laser Dynamics*
- *Numerical Mathematics and Scientific Computing*
- *Nonlinear Optimization and Inverse Problems*
- *Interacting Random Systems*
- *Stochastic Algorithms and Nonparametric Statistics*
- *Thermodynamic Modeling and Analysis of Phase Transitions*

3.1 Research Group *Partial Differential Equations*

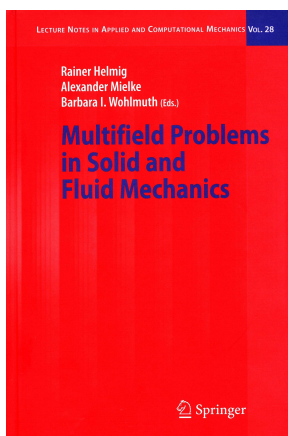
The main focus of this research group is the analytical understanding of partial differential equations. The theory is developed in close connection to well-chosen problems in applications, mainly in the following areas:

- Evolutionary systems with nonlocal interactions, in particular, with applications in semiconductor device modeling and in phase separation problems
- Modeling of optoelectronic devices including quantum effects
- Multifunctional materials

The mathematical methods range from pure functional analysis and mathematical physics to modeling and numerical methods:

- Existence, uniqueness, and regularity theory for initial and boundary value problems in non-smooth domains and with nonsmooth coefficients
- Coupling of different models, in particular, using models accounting for nonlocal interactions
- Iterative and variational methods using energetic formulations that are based on physically motivated functionals
- Qualitative methods for evolutionary systems
- Multiscale methods for the derivation of effective models on larger scales from models on smaller scales

The study of the well-posedness of the underlying partial differential equations leads to a deeper understanding of the underlying physics and provides basic information for the construction of efficient numerical algorithms. In cooperation with other research groups, corresponding software tools are under development that will enable parameter studies or the optimization of technological products. For instance, the software package **WIAS-TeSCA**, which was developed in this research group, is used worldwide in industry and scientific institutes for the simulation of semiconductor devices.



The year 2006 marks the official end of several coordinated programs. First, there is to be mentioned the European Research Training Network “SMART SYSTEMS — New Materials, Adaptive Systems and their Nonlinearities: Modelling, Control and Numerical Simulation”, which started in November 2002. The final conference took place in Rome in October and was attended by the three young researchers Adrien Petrov, Florian Schmid, and Aida Timofte and the group leader. Moreover, the Collaborative Research Center SFB 404 “Multifield Problems in Solid and Fluid Mechanics” at Universität Stuttgart terminated after 12 successful years. The final report appeared as Volume 28 in the Series “Lecture Notes in Applied and Computational Mechanics” and was edited by R. Helmig (Stuttgart), A. Mielke (WIAS), and B. Wohlmuth (Stuttgart), cf. [1].

The Priority Program SPP 1095 “Analysis, Modeling and Simulation of Multiscale Problems” ended in 2006 with the “Conference on Multiscale Problems”, which was organized by F. Bornemann, S. Luckhaus, A. Mielke, S. Müller, and H. Spohn. It took place from October 9–11 at the Technische

Universität München and brought together leading scientists from all over the world as well as the German researchers on multiscale problems. The program started in 2000. It was supported by the German Research Foundation and coordinated by Alexander Mielke. A concise presentation of the achievements of the research done by the 23 projects within the Priority Program appeared in late September as the state-of-the-art volume “Analysis, Modeling and Simulation of Multiscale Problems” (cf. [4]). Two of the WIAS contributions (by research groups *Partial Differential Equations* and *Thermodynamic Modeling and Analysis of Phase Transitions*) are dedicated to the passage from discrete, atomistic models to continuum models described by partial differential equations, see also the Scientific Highlights article “Continuum Description of Discrete Lattice Models” on page 18.

Another topic in the above book addresses the modeling of semiconductor devices that is one of the central themes in this research group. The modeling basically distinguishes three spatial scales: the atomistic scale of the bulk semiconductor materials (sub-Angström), the scale of the interaction zone at the interface between two semiconductor materials together with the scale of the resulting size quantization (nanometer), and the scale of the device itself (micrometer). The work [2], which arose through a collaboration with the Research Group *Numerical Mathematics and Scientific Computing*, focuses on the two-scale transitions inherent in the hierarchy of scales in the device. It starts with the description of the band structure of the bulk material by $k \cdot p$ Hamiltonians on the atomistic scale by an obtained envelope-function approximation. However, this approximation may lead to spurious modes in the $k \cdot p$ Schrödinger model, which are inherited from anomalous band bending on the atomistic scale. We found reasonable conditions on the coefficients of the $k \cdot p$ Schrödinger operator that prevent spurious modes, and we derived efficient estimates on the size of the band gap. Using these results, it was possible to study the electronic band structure of strained quantum wells. Further, the assumption of flat-band conditions across the nanostructure allows for upscaling of quantum calculations to state equations for semiclassical models. For the $k \cdot p$ Schrödinger theory with low-gap quantum wells, we provide a proper rescaling of the optical matrix avoiding spurious modes.

Topics involving problems of continuum mechanics were studied in the the DFG Research Center MATHEON in the subproject C18 “Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys” as well as in the European Network “Smart Systems”. These projects mainly concern the modeling of multifunctional materials; cf. [5].

A breakthrough was also made in the context of fracture mechanics for finite-strain elasticity. The object of fracture mechanics is to describe the behavior of a body with a crack subjected to external loading. An important question is whether a pre-existing crack will grow for a given loading. Moreover, the form of the crack or its branching should be predicted.

Various fracture criteria are discussed in the literature, among which Griffith’s classical energy criterion is frequently used. This criterion states that an existing crack in an elastic body is stationary if the total potential energy in the current configuration is minimal compared to the total potential energy of all admissible neighboring configurations. In the simplest 2D case, where the crack is a part of a straight line (e.g., an interface) and where it can grow only straight ahead, the Griffith criterion can be reformulated in terms of the energy release rate (ERR). The ERR is defined as the

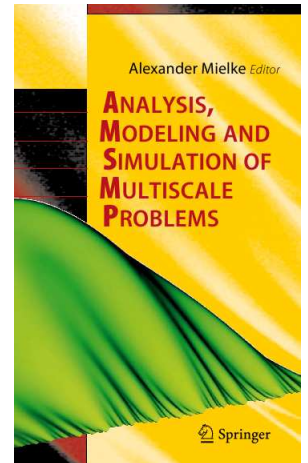
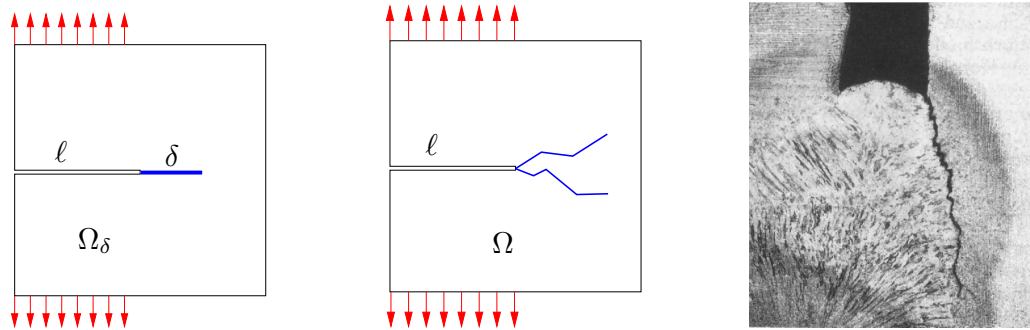


Fig. 1: Left: straight growing crack. Middle: branched crack. Right: experimental picture of a crack starting at an inward-pointing corner of the domain (from Blumenauer, Pusch: *Technische Bruchmechanik*, Deutscher Verlag für Grundstoffindustrie, Leipzig, Stuttgart, 1993)

derivative of the elastic deformation energy with respect to the crack length.



Based on this definition, we have established a formula for the ERR in the case of finite-strain elasticity assuming that the elastic energy density is given by a polyconvex function [3]. We showed that the ERR can be expressed via the Griffith formula, which is based on Eshelby tensors, and by the J -integral. As a mathematical tool, we proved a theorem that guarantees the weak convergence of the corresponding Eshelby tensors, if the minimizers converge weakly and if the energies converge. Since minimizers may be nonunique, one can give two different interpretations of what is meant by “admissible neighboring configuration” in the Griffith criterion: Is it sufficient that the different cracked domains are “close” to each other or does one also require that minimizers on domains with extended cracks are “close” to a particular minimizer on the original domain? These different interpretations are reflected in our formulas for the ERR and are an essential difference between the finite-strain case and the case of linear elasticity.

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3.2 Research Group *Laser Dynamics*

The research of this group is devoted to the development of mathematical methods and theories in the field of nonlinear dynamics, with applications especially in optoelectronics. The main topics in 2006 were:

- Dynamics of multisection semiconductor lasers
- Pulses in nonlinear optical media.

The research related to these topics includes mathematical modeling, theoretical research on dynamical systems occurring in laser theory and nonlinear optics, numerical implementation, and device simulation.



Fig. 1: Participants of the 6th Crimean School and Workshop “Nonlinear Dynamics, Chaos, and Applications”

A major event in the year 2006 was the Workshop “Complex Dynamics and Delay Effects in Coupled Systems”, organized at Humboldt University within the framework of the DFG Collaborative Research Center 555 “Complex Nonlinear Processes”. In this interdisciplinary workshop with about 100 participants from 15 countries, leading experts from mathematics, physics, and applications in optoelectronics and neuroscience came together to present and to discuss recent results and developments in this very active field of research. Further important events were the 6th Crimean School and Workshop “Nonlinear Dynamics, Chaos, and Applications: From Laser to Brain, from Communication to Medicine”, where four talks were given by members of this research group, and the workshop “Nonlinear Dynamics in Modelocked Lasers and Optical Fibers” at WIAS; see page 86.

In 2006, two funded projects were completed successfully:

- Within the project diMOLA on directly modulated lasers in cooperation with Fraunhofer-Institut Nachrichtentechnik Heinrich-Hertz-Institut (HHI) and Research Group *Partial Differential Equations*, a new device concept for direct signal modulation at 40 GBit/s has been developed theoretically, and, after successful experimental realization, [1], submitted for patent protection.
- The main results of the project on mode-locking in lasers with saturable absorbers, which was supported within the research network Terabit Optics Berlin, was a new modeling approach to mode-locking in the framework of delay-differential equations. It has been used successfully

for both theoretical investigations of mode-locking dynamics and their instabilities and an optimization of the devices, developed by our project partners at HHI, [2]. Recently, this approach has been successfully adapted to mode-locked quantum-dot lasers [3], which offers the possibility for further important applications.

Furthermore, the progress in the following fields of research is to be mentioned:

Numerical methods for laser dynamics

The software package `LDSL-tool` has been extended by several post-processing routines allowing an automatic characterization of the computed transient regimes and an estimation of the synchronization quality of coupled laser devices. For this purpose, the regularity of various filtered transients in time and frequency domains was estimated, auto- and cross-correlation functions were analyzed, the corresponding finite-dimensional mode approximation systems were constructed, and some largest Lyapunov exponents therein were estimated. All these new routines were used for an automatic identification of chaotic regimes as well as for the identification of parameter regions with optimum contrast between the synchronized/desynchronized chaotic states. This topic is especially interesting for the secure data transmission in optical communication systems; see [4].

Dynamics of laser systems with delayed coupling or feedback

Within this project, which is founded by the DFG Collaborative Research Center SFB 555 “Complex Nonlinear Processes”, bifurcation theory for delay-differential equations with large delay has been developed, [5], and applied to the time-delay autosynchronization problem (Pyragas control). Dynamical scenarios in a large array of coupled semiconductor lasers have been studied. Lyapunov exponents in periodically forced chaotic oscillators were also theoretically investigated.

Pulses in nonlinear optical media

This project was supported within the research network Terabit Optics Berlin. The generation of stable high-repetition-rate trains of femtosecond optical pulses was investigated by taking advantage of the nonlinear properties of optical fibers. On the base of an extended nonlinear Schrödinger equation, broadband continua generated in highly nonlinear dispersion-flattened fibers were investigated, with subsequent compression in standard single-mode fibers. Beyond critical pulse powers, a fundamental compression limit by pulse splitting was discovered, leading to a complete breakdown of this compression scheme. Experiments by the cooperation partner HHI substantiated the investigations; see [6]. The impact of pulse and fiber parameters on the pulse splitting has been analyzed in detail.

Localization of light in nonlinear photonic crystal materials

Properties and bifurcations of Bragg-localized structures of light were studied in a wide-aperture nonlinear optical cavity with intracavity photonic crystal film; cf. [7]. The conditions for the existence and stability of stationary Bragg-localized structures and a transition to a localized structure moving in the transverse direction were analyzed.

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3.3 Research Group *Numerical Mathematics and Scientific Computing*

The mathematical description of a significant number of scientific and technological problems leads to *differential equations* that describe temporal, resp. spatial variations of the state of the corresponding physical system. Typically, these equations cannot be solved in closed form, and *numerical methods* have to be applied to calculate *approximate solutions*.

Numerical methods for systems of differential–algebraic equations (DAEs)

Systems of DAEs, i.e., of ordinary differential equations and additional algebraic equations, are used in situations when the spatial structure of the problem is not present or can be ignored. Among many other problems, electrical networks and processes in chemical plants can be modeled by this type of description. Based on a modular approach, the simulator BOP uses divide-and-conquer techniques to enable efficient steady-state, transient, as well as Monte Carlo simulations for such systems. BOP 2.2 is currently used for industrial gas turbine simulation at ALSTOM Power (Switzerland) Ltd.

The new release BOP 2.3 will be delivered soon, and improves:

- Steady-state simulation mode
- Simulation control and result evaluation
- Modeling language
- Transient as well as Monte Carlo simulation mode

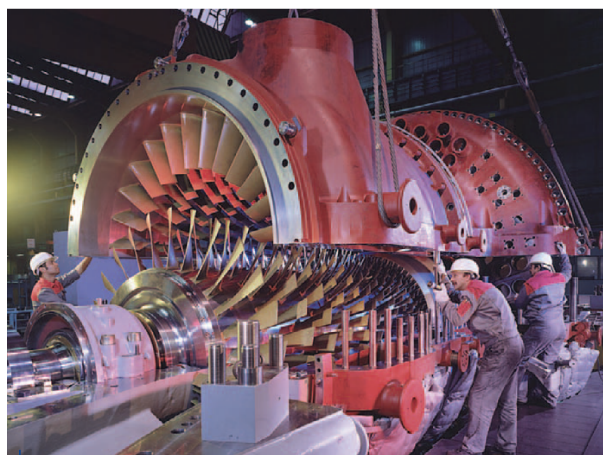


Fig. 1: Assembly of a gas turbine
(source: ALSTOM Power Ltd.)

Numerical methods for systems of partial differential equations (PDEs)

Partial differential equations are used to model problems where the spatial structure of the model has to be taken into consideration. Within the large class of problems of this type, the main applications of the group are semiconductor device problems and transport problems in porous media. The unknowns in PDEs are functions of one or several spatial variables and, possibly, of time. Computers can represent them only approximately. There are several possibilities to generate such approximations.

Concerning the discretization of PDEs, the focus of the group is on finite volume methods that are able to preserve qualitative properties of the problem (L^∞ -bounds, dissipativity, etc.). Every unknown function is approximated by its average over the control volume. By integrating the partial differential equation, and using Gauss's theorem, it is possible to calculate the rate of exchange with the neighboring control volumes. This results in a large system of linear (or nonlinear) equations, at least as many as control volumes, which may count in hundreds of thousands.

Therefore, the process of creating a simulation model is connected with a number of steps to be performed. Among them are

- Derivation of the model
- Mesh generation
- Study of the convergence of the discrete problem to the continuous one
- Solution of the arising nonlinear and linear systems of equations
- Implementation in software
- Post-processing and visualization

3D semiconductor device simulation

The work on 3D semiconductor simulation focused on semiconductor photon detectors and on avalanche generation.

Semiconductor photon detectors are highly sensitive devices using the Depleted P-channel Field Effect Transistor (DEPFET) principle in order to integrate a first amplification stage into the photon detector for each pixel. Such detectors are planned to provide the sensor technology for a space-based X-ray telescope. Future medical imaging systems could profit from such a design as well. In cooperation with R. Richter (Semiconductor Laboratory, Max Planck Institute (MPI) for Physics, Munich, and MPI for Extraterrestrial Physics, Garching), the system of semiconductor device equations is solved in a three-dimensional domain representing a DEPFET sensor cell [3].

It is possible now to simulate a few elementary cells of an infinite grid to study symmetry breaking and filament formation due to avalanche generation in highly symmetric 3D structures. In addition to direct connections to existence and convergence theory of discrete solutions, solution techniques for the linearized problem are a crucial issue. Figures 2–4 display cut and isosurface views of a CoolMOS-like structure with 16 elementary cells showing symmetry breaking at avalanche

breakdown. With increasing cell numbers, the breakdown is moving to lower voltages, and one elementary cell group carries most of the current.

Furthermore, precise contact current evaluation based on adjoint techniques and a weak discrete formulation has been studied. It could be shown that second-order contact current errors result from first-order errors in the solutions of the original problem and its adjoint; see [2].

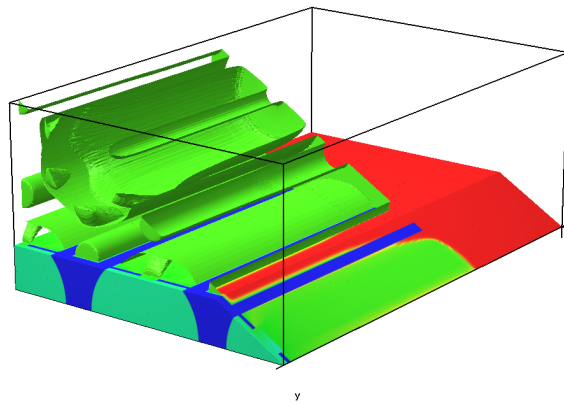


Fig. 2: Electron density in a CoolMOS-like device

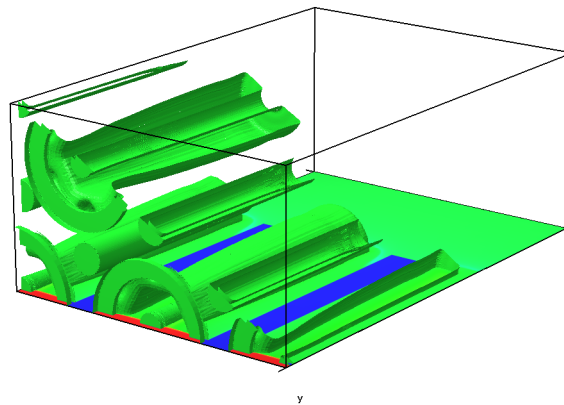


Fig. 3: Hole density in a CoolMOS-like device

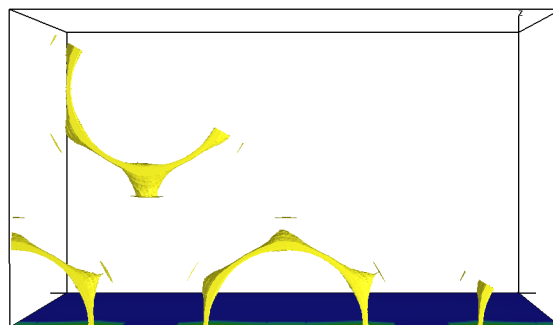


Fig. 4: Avalanche generation rate in a CoolMOS-like device. The symmetry-breaking effect is clearly visible.

Modeling of biased multi-quantum-well structures

Biased multi-quantum-well structures are used in Mach–Zehnder modulators for fiber optical telecommunications systems in order to achieve a field-dependent change of the refractive index. The electric field in quantum wells leads to a shift of the transition energies (quantum-confined Stark effect) and a modification of the transition matrix elements (Figure 5). Both effects lead to a change of the position and the height of the absorption and thus to the change of the refractive index. In a project funded by the DFG (Priority Program SPP 1095 “Analysis, Modeling, and Simulation of Multiscale Problems”), the group investigated the field dependence of the transition energies and the transition matrix elements for an example InGaAsP quantum-well lattice matched to InP by eight-band $k \cdot p$ calculations of the electronic states with **WIAS-QW** [4]. Using the numerical model **WIAS-QW**, more comprehensive simulations have been carried out at the Heinrich Hertz Institute, Berlin, of the Fraunhofer Gesellschaft, in order to optimize the performance of the modulation behavior of the multi-quantum-well structure.

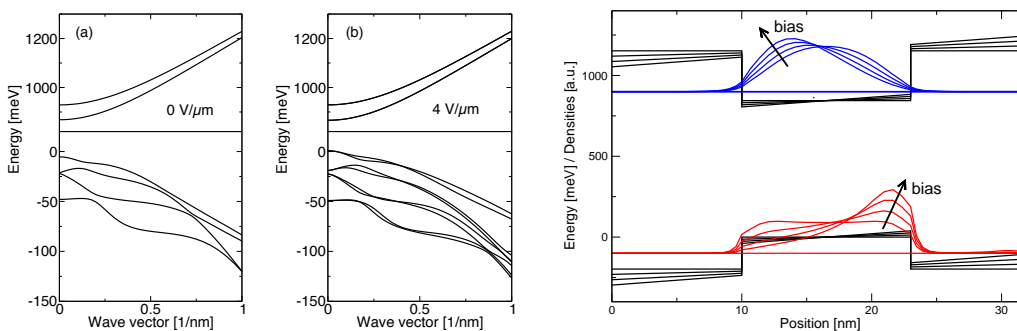


Fig. 5: Band structure and electronic states in a InGaAsP-InP lattice-matched biased quantum well. The electrons are pushed to the left, and the holes are pushed to the right, resulting in a reduced transition matrix element.

Modeling of electrochemical flow cells

Direct methanol micro fuel cells (DMFCs) are possible candidates for replacing rechargeable batteries in cell phones, laptops, and other small devices by a system with significantly higher capacity. Mathematical and numerical modeling allows for a better understanding of the complex transport and reaction phenomena in such a cell. The group coordinates the joint project “Modeling, Experimental Investigation and Numerical Simulation of Direct Methanol Micro Fuel Cells” funded by the German Federal Ministry of Education and Research (BMBF). The focus has been on the development and implementation of a coupled model of transport and electrochemical reactions in a flow cell suited for differential electrochemical mass spectroscopy (DEMS). The aim of this work is the support of the theoretical interpretation of measurements of methanol kinetics by numerical simulation. A comprehensive model for methanol kinetics is important for the understanding of the functioning of DMFCs.

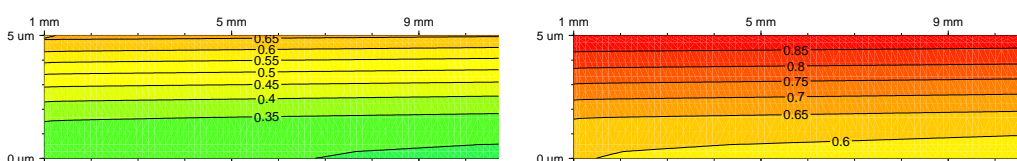
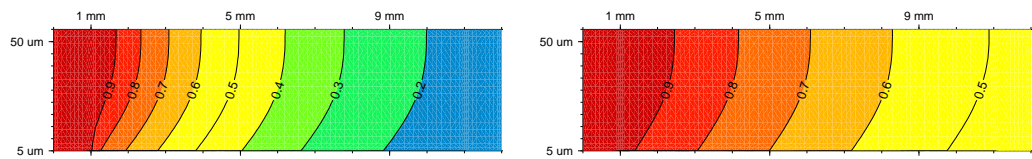


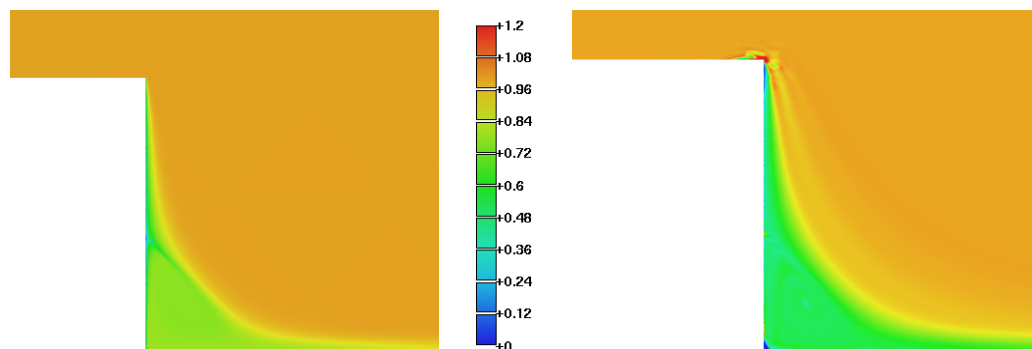
Fig. 6: Adsorbed CO concentration (normalized) in the porous catalyst region of a DEMS cell after 200 s (left) and 400 s (right) of a CO poisoning process

Fig. 7: Dissolved hydrogen concentration (mol/l) in the flow region of a DEMS cell after 200 s (left) and 400 s (right) of a CO poisoning process



The convergence of the finite volume method used for the discretization of species transport – e.g., in the flow region of a the DEMS cell – is based on the assumption that the convective field and its discrete counterpart are divergence-free, modeling a mass conservative flow. If the convective field arises from the approximate solution of the Navier–Stokes equations, the compliance with this condition is a topic of active research. A finite element discretization of the incompressible Navier–Stokes equation is studied, which uses the Scott–Vogelius element [1]. The finite element space generated by this element allows for pointwise divergence-free solutions of the incompressible Navier–Stokes equations. The examination of this property in the coupling with a convective flow problem is currently under consideration.

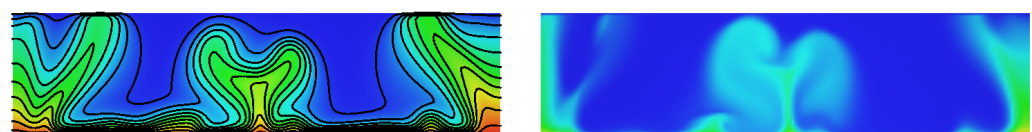
Fig. 8: Convective transport behind a backward-facing step: stable solution with divergence-free discrete flow field (left), transport of density error generated by a non-divergence-free solution of the Navier–Stokes equations (right)



Qualitative state of thermohaline flow in the subsurface

The process of thermohaline convection in the subsurface can be described by a nonlinearly coupled system of three PDEs, describing water flux, heat transport, and transport of salt dissolved in water. In a project supported by the DFG (Priority Program SPP 1135 “Dynamics of Sedimentary Systems under Varying Stress Regimes: The Example of the Central European Basin”), based on the `pdelib` toolbox, a finite-volume-based numerical model has been coupled with a module for Lyapunov exponent estimation based on tracing the evolution of perturbations of the initial state using the implicit Euler method. The goal is the utilization of this information for the discrimination of possibly chaotic flow behavior and the comparison of simulations of chaotic flow on different discretization grids.

Fig. 9: “Chaotic” temperature movement driven by heating from below in a layer of cenozoic sediment (left). Driven by thermal convection, salt is transported in plumes to the top. The tips of these plumes show a seemingly random movement along the surface (right).



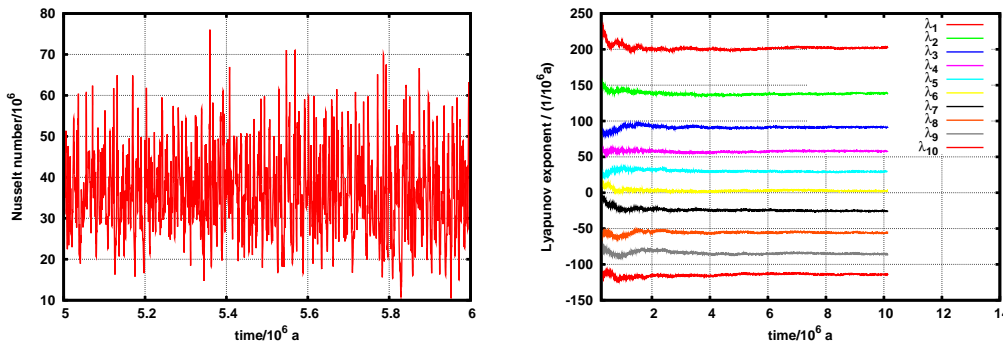


Fig. 10: The time series of the Nusselt number shows erratic behavior (left). Estimating Lyapunov exponents numerically results in five positive ones, indicating a chaotic state of the system (right).

Sparse direct solver PARDISO

The PARDISO project in collaboration with O. Schenk (University of Basel) has been continued. It is aimed at the further development of algorithms and software for the numerical solution of large sparse linear systems by the Gauss method tuned in such a way that it runs efficiently on shared-memory parallel computers. The focus on this architecture allows to utilize the OpenMP parallel programming directives, which results in an efficient implementation of parallel algorithms both with respect to performance on target machines and with respect to coding. With these advantages, the growing availability of multicore processors for general-purpose computers and the integration of OpenMP into the GNU compiler suite, one can expect that this programming paradigm will find a larger audience than ever before. The current focus in the development of PARDISO is on extended pivoting, and on saddle point and symmetric indefinite problems. In the result, the code can be applied reliably to a wider class of problems; see [5].

Three-dimensional boundary conforming Delaunay mesh generation (TetGen)

Details about this project can be found in the Scientific Highlights article “The TetGen Project” on page 38.

Software environment for the numerical solution of PDEs: `pdelib2`

A software environment is maintained where necessary components for the creation of simulators based on PDE models are made available for applied projects. Its data structures are based on multidimensional arrays. These arrays are used to store solutions, grids, matrices, and other objects. The user can directly access the grid generators triangle (J. Shewchuk) and TetGen. For parallel computations, the generated grids are partitioned using METIS. The linear algebra subroutines and the programming interfaces for matrix assembly and nonlinear operator application support parallel implementations for shared memory computers. Various Newton methods for the solution of nonlinear problems are available. The resulting linear problems are solved by iterative and direct solvers. For data description and solution control, a large part of the programming interface has been made accessible from the extension language Lua. The visualization of the computed

data may be performed using OpenGL. Finally, graphical user interfaces for specialized problems can be designed using the FLTK toolkit. The code is portable among Linux, UNIX servers, MacOS X, and Microsoft Windows.

Current work is focusing on the addition of features important for the support of several other projects. Among them are

- Impedance calculations for coupled systems of reaction-diffusion-convection systems
- Lyapunov exponent estimate during implicit time stepping
- Additions to the API necessary for the creation of flexible user interfaces, as Lua-Terminal and stdio-redirection, event-oriented signal-slot concept Lua-based persistent dynamic containers
- Visualization of vector fields

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3.4 Research Group *Nonlinear Optimization and Inverse Problems*

The research group studies the optimization of structures and processes, and their interaction. The tasks range from basic research on the formulation, analysis, and numerics of the optimization problems to the development and implementation of efficient numerical algorithms. Special emphasis is laid on the solution of real-world problems in cooperation with partners from industry and from the applied sciences. The work is supported by public and industrial funding.

In 2006, the research group has acquired two new externally funded projects. In a joint work with T. Stykel (Technische Universität Berlin) within the DFG Research Center MATHEON, the focus is on reduced-order modeling and optimal control of multibody systems coupled with a parabolic evolution equation. Within the new DFG Priority Program SPP 1204 “Algorithms for the Fast Design and Analysis of Process Chains in Deformation Technology”, the identification of material parameters and the optimal control of the cooling track after hot rolling of new multiphase steels will be investigated together with W. Bleck (RWTH Aachen).

In continuation of their successful work in the fields

- Optimization and inverse problems in diffractive optics and electromagnetics
- Optimal control of production processes

the group has made significant progress in their research program, which will be explained in more detail below. An overview of new results for optimization problems subject to chance constraints can be found in the Scientific Highlights article “Optimization Problems with Random Constraints” by René Henrion on page 27.

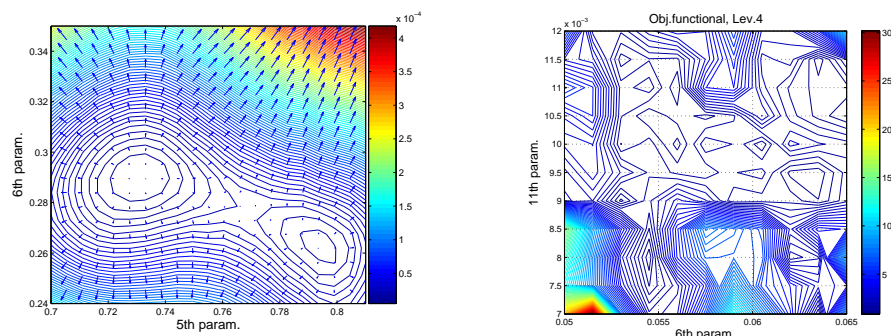
The group is collaborating on joint projects with other research groups at WIAS concerning optimal control of coupled electrothermal models and optimal regularity for elliptic and parabolic operators (with Research Group *Partial Differential Equations*), numerical approximation of thermomechanical models within `pdelib` and the development of a graphical user interface for the generation of geometries within `DiPoG-2.1` (with Research Group *Numerical Mathematics and Scientific Computing*), and the modeling of phase transitions (with Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*).

Optimization and inverse problems in diffractive optics and electromagnetics

The optimization part of the program package `DiPoG-2.1` provides an appropriate tool for the inverse problem of scatterometry. Here, geometry and material parameters of test configurations like multilayered line/space structures with different sidewall angles are to be recovered from the scattered light fields incited by plane-wave illumination (cf. [2]). More precisely, the deviation of measured efficiency values from simulated values is to be minimized, i.e., an objective functional

in form of a weighted least-squares sum is to be optimized. In cooperation with Physikalisch-Technische Bundesanstalt (PTB), DiP_{OG} has been applied to the reconstruction of chrome-on-glass masks in lithography. To determine optimal measurement settings, a new tool for the sensitivity analysis has been developed, which has turned out to be very useful for the analysis of these masks (cf. [3] and see the two-dimensional example of an objective functional on the left in Figure 1). Moreover, the investigation of more challenging masks of the next generation, the so-called *EUV masks*, has been started. A sensitivity analysis for the design of measurement and a good scaling will be needed to avoid situations as depicted in Figure 1, right, where large numbers of local minima hinder the reconstruction.

Fig. 1: Two geometry parameters, left: chrome-on-glass masks with moderate ratio period over wavelength. Right: EUV masks with larger ratio period over wavelength



If the periodic cross section of an optical grating is determined by one or two simple profile curves, then the best method of computation for the electromagnetic field is likely to be an integral equation approach. In [7], the theoretical foundation of a fast realization of an integral equation method is presented, which is based on the spline collocation adapted to corner profiles and thin coated layers. A considerable reduction of computing resources is obtained by using graded meshes on the boundary, exponentially converging quadrature formulas for nearly singular integrals, a new representation of the periodic Green function by the Faddeeva function, and a preconditioned GMRES for solving the linear system with dense unsymmetric matrices. The method is implemented in the program package IESMP, used by WIAS's cooperation partner Carl Zeiss Oberkochen, and outperforms other methods for the simulation of diffractive structures with nonsmooth profiles and thin layers.

Extending the previous work on inverse diffraction problems, an investigation of inverse problems for fluid-solid interactions, which recently have received much attention in the engineering literature, has been started. To reconstruct the shape of the elastic scatterer from a knowledge of the far-field pattern of the fluid pressure, this highly ill-posed problem is reformulated as a nonlinear optimization problem including regularization terms. Convergence results for the reconstruction method could be obtained as well as gradient-based algorithms to minimize the corresponding cost functionals. The analysis relies heavily on a new variational approach to the direct transmission problem involving nonlocal boundary conditions; cf. [1].

Optimal control of production processes

From the mathematical point of view, the main focus of research in 2006 lay on the treatment of optimal control problems with pointwise state constraints and the analysis of multifield problems.

In [6], for the first time, error estimates for a fully discretized linear-quadratic problem with pointwise state constraints are discussed. The obtained results are optimal in view of the low regularity of the optimal solution. Furthermore, in cooperation with M. Hinze (Universität Hamburg), a Lavrentiev regularization of a linear quadratic state-constrained problem has been considered, which was approximated by a semi-discretization in the spirit of [4]. Based on convergence results for the Lagrange multipliers, it was possible to derive the superconvergence properties already known from the control-constrained case [5].

In cooperation with J. Rehberg (Research Group *Partial Differential Equations*), an investigation of the thermistor problem has been started. Relying on maximal regularity results for parabolic equations, the unique solvability of the state system has been proved. The corresponding state-constrained control problem is under study. The results, including numerical computations that are performed in cooperation with W. Ring (Universität Graz) will be completed in spring 2007.

Another multifield problem related to thermomechanical phase transition models as discussed in project C11 of the DFG Research Center MATHEON has been studied. It could be shown that the complete system of model equations admits a unique weak solution. The analysis relies heavily on regularity results for the quasi-static momentum balance. The result will be published in a forthcoming preprint.

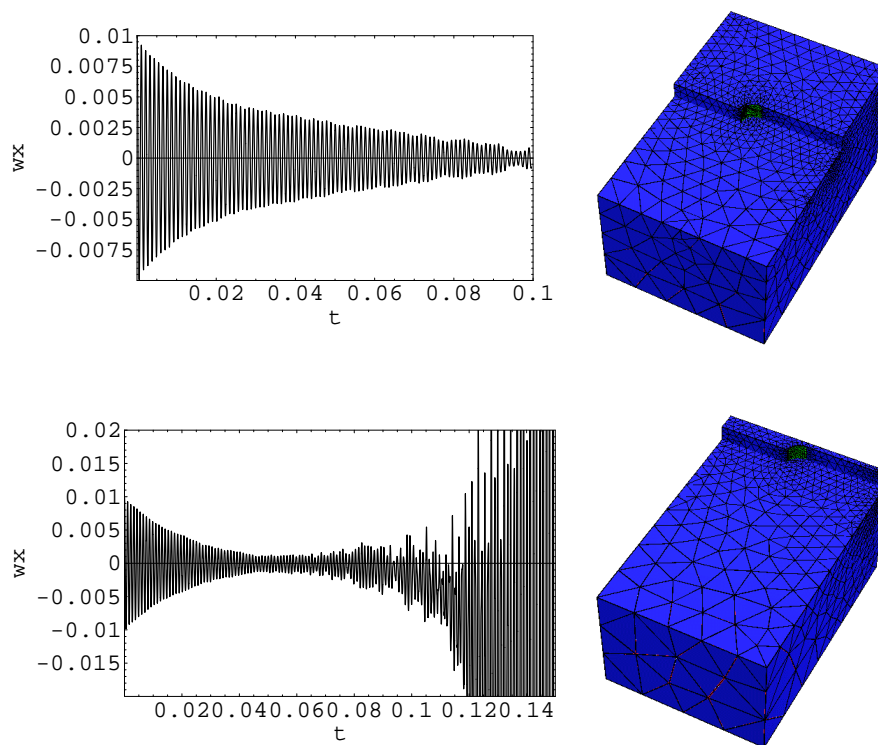


Fig. 2: Stabilizing (top) or destabilizing (bottom) effect of interaction between process and structure in high-speed milling

Finally, two exciting results related to applications in the control of production processes should be mentioned. In a project within the DFG Priority Program SPP 1180 “Prediction and Manipulation of Interaction between Structure and Process”, a model for the coupled description of process and structure in high-speed milling has been developed and implemented within `pdelib`. It was possible to demonstrate numerically that the workpiece may stabilize or destabilize the milling process depending on the workpiece stiffness (cf. Figure 2).

Remarkable progress has also been made in the industrially funded long-term research project on virtual production planning. In 2006, issues like task- and path-planning for cooperative robots were on the agenda. Figure 3 depicts a typical situation: A given set of weld points has to be assigned to two welding robots while the handling robot moves the workpiece from one pallet to another one.

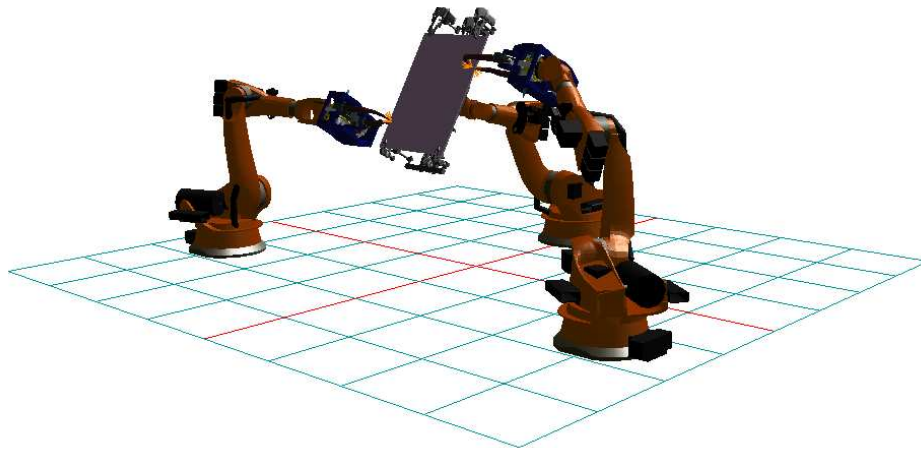


Fig. 3: Weld point assignment and path-planning for cooperative robots

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3.5 Research Group *Interacting Random Systems*

The research group *Interacting Random Systems* investigates microscopic stochastic models of complex systems arising from a variety of applications in the sciences, economics, and engineering. The main objectives are the rigorous derivation of macroscopic laws, the analysis of long-term behavior, and the development of stochastic numerical algorithms.

The year 2006 was marked by particular success in the context of funding for large-scale projects. Most importantly, the re-submitted application for an International Research Training Group “Stochastic Models of Complex Processes” (IRTG “SMCP”, jointly with Humboldt-Universität zu Berlin, Technische Universität Berlin, Universität Potsdam, University of Zurich, and ETH Zurich; coordinator: Anton Bovier) was approved on June 23 by the German Research Foundation DFG and received funding of approximately 1.5 million euro for an initial period of 4.5 years, starting October 1, 2006. This will finance 15 Ph.D. students and two postdoctoral researchers, and provide a rich training and research environment for all young researchers in probability theory in Berlin. Moreover, it will establish an international network for graduate education in applied probability, in which WIAS will play an important and visible rôle.

The opening of the IRTG “SMCP” was marked by a one-day opening colloquium held at WIAS on November 29, 2006, followed by a reception at the Swiss Embassy in Berlin.

The application by Anton Bovier and Dima Ioffe (Haifa) for a research grant with the German-Israeli Foundation on “Metastability and phase segregation” was approved, so that two such grants are now operational within this research group. The grant will fund as of January 1, 2007, one postdoctoral position and mutual travel for a period of three years.

Finally, Wolfgang Wagner and Hans Babovsky (Ilmenau) were awarded a DFG grant for a research project “Influence of spatial fluctuations on the gelation behavior of coagulation processes” for a two-year period.

The year 2006 was also noticeable for the change in the group’s composition, notably due to the fact that two of its permanent members left WIAS: Barbara Gentz received and accepted a call on an associate professorship at the University of Bielefeld and left WIAS in October (in the meantime, she also received an offer of a full professorship at the University of Tübingen). She has been a great asset for the group over the last years and has had an essential impact on the group’s research. Her success demonstrates the recognition of her work.

Klaus Fleischmann retired at the end of 2006. His research on superprocesses and interacting diffusions in the institute over the last 15 years has been a cornerstone of the work in this group and has greatly contributed to the standing of the group in the international community.

In addition, one of our postdoctoral researchers, Nicolas Champagnat, was offered a permanent research position with INRIA at Sophia Antipolis and left in August. During his stay as a postdoc, he initiated a very challenging program for studying the emergence of spatial structures in interacting population models. This will hopefully lead to a continuing collaboration with him now that he is back in France.

It will be a major challenge for the next year to replace these excellent researchers and to restructure the group.

To conclude the overview over last year's events, some highlights from research results are mentioned:

Coagulation processes

An essential step towards a more realistic modeling of coagulation phenomena involves the inclusion of spatial extension in stochastic particle models for coagulation processes. A particularly challenging task in this context is the study of the gelation phenomenon related to a phase transition due to very fast coagulation.

A two-site spatial coagulation model is considered in [1]. Particles located at the same site stick together at a rate proportional to the product of their masses. Independently, particles jump to the other site at a constant rate. A new effect of induced gelation is observed — gelation happening at the site with the larger initial number of monomers immediately induces gelation at the other site. The limiting behavior of the model is derived rigorously up to the gelation time, while the expected post-gelation behavior (one or two giant particles randomly jump between the two sites) is illustrated by a numerical simulation.

A coagulation model on a finite spatial grid is considered in [2]. Particles located at the same site stick together according to some coagulation kernel that grows sufficiently fast so that gelation is observed. Independently, particles jump randomly between sites. The jump rates are assumed to vanish with increasing particle masses so that the gel is immobile. The asymptotic behavior (for increasing particle numbers) of this model is characterized in terms of a nonlinear equation. Two aspects of the limiting equation are of special interest. First, for a certain class of coagulation kernels, this equation differs from a naive extension of Smoluchowski's coagulation equation. Second, due to spatial inhomogeneity, an equation for the time evolution of the gel mass density has to be added. Two different gel growth mechanisms (active and passive gel) are found depending on the type of the coagulation kernel.

Random walk in random scenery

In 2006, group members turned to this research topic of growing international interest. In [3] moderate deviation principles in all dimensions $d > 1$ were established, with precise asymptotics in dimensions $d > 4$. The proofs use new concentration inequalities for *self-intersection local times* of random walk, which are of independent interest.

Deviation behavior of Galton–Watson processes

Essential progress has been achieved. In [4], *lower deviation probabilities* were described for the whole class of supercritical Galton–Watson processes. This allowed to find the *fine asymptotics*

of large deviation probabilities for sums of i.i.d. random variables defined on Galton–Watson processes; see [5]. The latter problem has received a lot of attention in connection with polymerase chain reactions.

Likelihoods and Λ -coalescents

The great obsession of population genetics is to uncover the processes that shape variability in living populations. Coalescent processes are the stochastic tools to describe the genealogy of sampled individuals from such populations and the evolutionary forces acting on them. The standard model used in the past is Kingman's coalescent; more recently, a larger class of so-called Λ -coalescents has been introduced, whose new feature is to allow for multiple mergers. A major challenge is to infer the parameters of the best-fitting mechanism from experimental data using maximum likelihood estimators. Due to the complexity of the models, explicit calculations are only feasible for very small sample sizes, and thus in the literature, so far only methods based on (rather coarse) summary statistics have been employed.

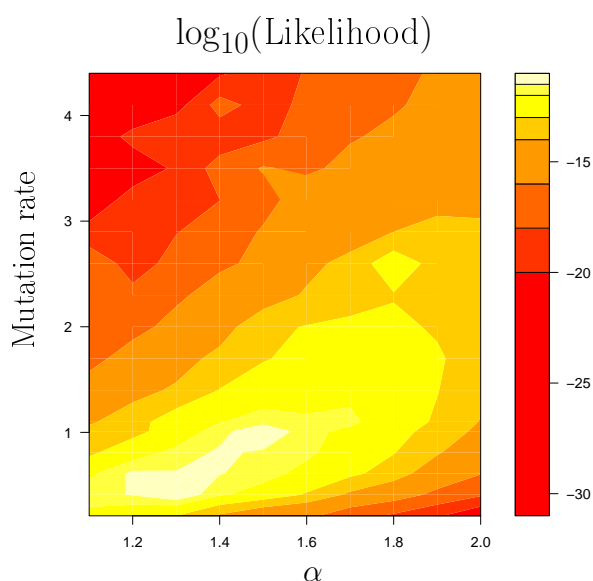


Fig. 1: Estimated (log-)likelihood surface for a sample of 117 Atlantic cod (referring to a 250 bp locus on the mitochondrial cytochrome *b* gene), a subsample of the sample described in E. Árnason, Genetics **66**:1871–1885. Abscissa: offspring distribution tail parameter α , ordinate: mutation rate. Maximum at (1.3, 0.5).

A Monte Carlo algorithm was developed that allows approximate integration over the high-dimensional space of genealogical trees connecting the sample and thus yields estimates for the desired likelihood. This algorithm was implemented in the program beta gene tree. Observations from Atlantic cod and HIV indicate that beta coalescents (a particular subclass of Λ -coalescents) are relevant for population genetic questions concerning marine species and viruses [6].

Stochastic models for spatially extended populations

A key question in population dynamics is whether and how spatial distribution is essential for survival of competing species. A model for a randomly reproducing, spatially extended population with local density-dependent feedback effects was studied. Additionally, a two-type version was considered, where the two species compete for local resources. Survival of the system and existence of a unique non-trivial equilibrium was proved as well as complete convergence (in that part of the parameter space where the corresponding deterministic, space-less system has a unique attracting fixed point, and when competition is sufficiently weak). Thus, local and global survival are equivalent in this regime. This is plausible in view of the biological interpretation, the obtained result is the first rigorous mathematical theorem for a stochastic model from this class [7].

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3.6 Research Group *Stochastic Algorithms and Nonparametric Statistics*

The research of the group is organized in the research projects *Statistical data analysis* and *Applied financial mathematics and stochastic simulation*, and focuses on problems from applied stochastics and financial mathematics.

The group's theoretical interests center around topics in applied and algorithmic probability theory and mathematical statistics that include methodological and theoretical aspects of statistical and numerical problems. This is complemented by investigations of their complexity.

The focus is on applications in economics, financial engineering, life sciences, and mathematical physics. Of special interest are the modeling of complex systems using methods from nonparametric statistics, risk assessment, and the valuation in financial markets using efficient stochastic algorithms. The developed methods find applications also in environmental research.

The research group has reached an internationally leading position with important mathematical contributions and the development of statistical software. Vladimir Spokoiny has almost completed his monograph *Local Parametric Methods in Nonparametric Estimation*, to appear in the Springer Series in Statistics.

Part of the research is carried out within the projects A3, A10, and E5 in the DFG Research Center MATHEON, within project B5 in the DFG Collaborative Research Center SFB 649 "Economic Risk", and within one project in the DFG Priority Program SPP 1114 "Structure Adaptive Smoothing Procedures with Applications in Imaging and Functional MRI". Members of the group were involved in several industrial contracts. New pricing methods for Bermudan products have led to a continued cooperation with the Landesbank Berlin Holding AG (former Bankgesellschaft Berlin AG). The group also participates in a contract with ALSTOM (Switzerland) Ltd., Baden on gas turbine process simulation. The contribution concentrates on general statistical modeling and Monte Carlo approximations.

In the following, some scientific highlights achieved by the research group in 2006 are detailed.

Statistical data analysis

Significant progress was made in the theoretical foundation of *structural adaptive smoothing methods*. The new formal concept of *Propagation and Separation* allows for the selection of critical parameters for the different adaptive procedures developed within this project, i.e., adaptive weights smoothing [2], stagewise aggregation, and pointwise adaptive procedures, by a common criterion. This allowed to obtain similar theoretical results for all three types of algorithms. In addition to the local polynomial and one-parameter local likelihood models considered before, the class of models that can be handled by these approaches has been extended to include local generalized linear models. A monograph, [1], is in preparation.

The structural adaptive methods for image denoising are now implemented as a package for the

R statistical system that allows to process grey value, color images with colored noise, and mean depending variance. Image denoising is based on one-parameter local likelihood models and local polynomial models.

Essential progress has been made in some exciting applications. Within the project *Image and signal processing in medicine and biosciences (A3)* in the DFG Research Center MATHEON, Karsten Tabelow and Jörg Polzehl completed a package for the R statistical system that allows to analyze a broad class of fMRI experiments. A corresponding conceptual paper has been published in *Neuroimage*, [3]. Two joint papers with partners from Cornell University on specific applications have been submitted. Further research includes specific problems in high-resolution fMRI and event-related fMRI experiments. The latter is based on identification of non-Gaussian components, [4]. A first approach for adaptive smoothing in diffusion tensor imaging (DTI) has been successfully tested. Work on tomography problems, e.g., from CT and small-angle tomography, was started.

A second project (A10) within MATHEON concentrates on *automatic model reduction for complex dynamical systems*. An algorithmic iterative method to estimate the effective dimension reduction (EDR) subspace of real-world stationary molecular systems was developed, which captures their conformational changes. It turned out that this semi-parametric dimension reduction method is able to detect conformational changes in medium-sized oligo-peptides, in good agreement with the computational results for tri- and penta-alanine. The results are reliable even if the conformational changes are rare events on the scale of the complete time series or if the dimension of the state space increases up to 84 in case of B-DNA.

Research within project B5 of SFB 649 focuses on effective dimension reductions for high-dimensional data and nonstationary time series.

Applied mathematical finance and stochastic simulation

The central theme of this project is the quantitative treatment of problems raised by industry, based on innovative methods and algorithms developed in accordance with fundamental stochastic principles. The project concentrates on two main areas: *applications in financial industry* and *computational physics*.

Stochastic modeling in finance

The new policy iteration method for solving Bermudan stopping problems, a key development in 2004–2005 in the context of *stochastic modeling in finance* (Kolodko and Schoenmakers), has been extended in [5] to problems with multiple exercise possibilities and in a forthcoming paper improved regarding computational efficiency. In this report, the broad reach of the iteration procedure is depicted in the Scientific Highlights article “Iterating Cancelable Snowballs and Related Exotics” on page 44. The development of an innovative generic Monte Carlo procedure for computing price upper bounds for Bermudan products by Belomestny, Bender, and Schoenmakers is considered a key result of the present period. As a main advantage, the perennial problem of time-consuming nested Monte Carlo simulation connected with the computation of these upper bounds is eliminated via an elegant regression procedure for the estimation of hedge martingales. Particularly, the upper bounds for American/Bermudan options based on considering consumption

processes developed in [6] in the preceding years, could be improved considerably in this way. In addition to the pricing of financial derivatives, the evaluation of sensitivities (“Greeks”) is also very important, in particular, for hedging. In this context, new probabilistic representations involving WKB (Wentzel, Kramers, and Brillion) approximations of Greenian kernels are developed by Kampen, Kolodko, and Schoenmakers. These representations allow for efficient Monte Carlo estimations of “Greeks” in high-dimensional problems. For various interest rate derivatives, the Libor rate model and its calibration is of main importance. In this area, the challenging research on jump-diffusion Libor models and other extensions is continued in the present report period. Further, in a study that is more on the theoretical side, by Bender (jointly with Sottinen and Valkeila), the theory of no-arbitrage pricing is pushed beyond the standard semi-martingale setting.

In the field of *stochastic models and algorithms in computational physics*, considerable progress has been achieved both in the theoretical development of new stochastic methods for solving boundary value problems and random field simulation, and in different interesting applications like faceted island formation in a crystal growth process, elastic body deformations under random loads, aerosol concentration, and flux footprint modeling in the problem of particle transport in the canopy.

An efficient stochastic algorithm based on the Random Walk on Spheres method for solving elasticity problems with random loads has been developed in [7].

An interesting practical problem of faceted island formation in a crystal growth process, known as Lifschitz–Slyozov–Wagner process, was solved [8], where a new type of island formation and growth was found. This work is carried out jointly with the Paul-Drude-Institut für Festkörperphysik, Berlin. A further study has been recently finished (see V.M. Kaganer, W. Braun, K.K. Sabelfeld: Ostwald ripening of faceted 2D islands, *Physical Review B*, in press).

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3.7 Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*

The research group studies initial-boundary value problems for nonlinear PDE and ODE systems that are related to phase transitions occurring in nature and in modern materials. The main focus is on multiscale modeling with strong coupling between thermodynamics, mechanics, analysis, and numerical simulations. In 2006 the research group continued most of the research lines from 2005. Additionally new topics have been started, viz.

- For the simulation of the growth of nano crystals and quantum dots, a new Cahn–Hilliard (CH) equation is modeled that differs from the convective CH equation by two orders in the regularizing term.
- Modeling of extended Cahn–Hilliard equations with strain-dependent surface tension for simulations and design of a new generation of solder joints in microelectronic devices
- Analysis and simulations of a coupled process involving heat conduction and flow in a changing magnetic field to control the flow pattern in a rotating liquid metallic melt
- Modeling and simulation of thin film flow along vertically rotating surfaces
- Analysis of nonlocal phase field systems with phase-dependent specific heat
- Modeling and analysis of discrete nucleation models and their continuum limits based on the Becker–Döring process

These new topics and those remaining from 2005 are related to interdisciplinary studies with industrial companies, external research groups from universities, external research institutes, and cooperations within WIAS with the research groups *Partial Differential Equations* (on continuum limits of discrete lattice models and on nonlinear elasticity), *Numerical Mathematics and Scientific Computing* (on bubble formation in direct methanol fuel cells), and *Nonlinear Optimization and Inverse Problems* (on precipitation phenomena in steel). A joint paper by W. Dreyer, M. Herrmann (Humboldt-Universität zu Berlin (HU)) and A. Mielke, “Micro-macro transition in the atomic chain via Whitham’s modulation equations”, [5], was selected by the Institute of Physics Publishing for inclusion in IOP Select, which is a special collection of journal articles based on the criteria: substantial advances or significant breakthroughs, a high degree of novelty, significant impact on future research.

In the above context of research topics, group members jointly with other partners conduct and supervise thirteen Ph.D. studies. These are partly carried out within the Graduate School GRK 1128 “Analysis, Numerics, and Optimization of Multiphase Problems”, and within the DFG Research Center MATHEON “Mathematics for key technologies”. The following list gives current objectives, institutions, and supervisors.

- Existence and uniqueness of a local phase field system with thermomechanical coupling (GRK 1128, Dreyer/Sprekels)
- Modeling, numerics, and experimental validation of a local phase field system with thermomechanical coupling (Technical University of Berlin (TU), Dreyer/Müller (TU))

- Modeling, analysis, and numerics of precipitation phenomena in steel (GRK 1128, Dreyer/Hömborg)
- Modeling, analysis, and numerics of nucleation and evolution of bubbles in ternary mixtures in direct methanol fuel cells (GRK 1128, Dreyer/Fuhrmann)
- Coarsening of dewetted liquid droplets (GRK 1128, Wagner/Recke (HU))
- Numerics of Navier–Stokes equations (industrial collaboration with funding, Münch/Niethammer (HU))
- Evolution of quantum dots with extended Cahn–Hilliard equations (MATHEON Project C10, Münch/Wagner)
- Modeling, asymptotic analysis, and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces (MATHEON Project C10, Münch/Wagner)
- Existence, uniqueness, and numerical simulations of the discrete Becker–Döring system and its continuous limit (MATHEON Project C14, industrial collaboration with funding, Dreyer/Niethammer (HU))
- Homogenization of a free boundary problem for the evolution of liquid precipitates in crystalline gallium arsenide (MATHEON Project C14, Dreyer/Niethammer (HU))
- Existence and uniqueness of a magnetohydrodynamical system with heat conduction (WIAS, Sprekels)
- Rigorous limits from 3D nonlinear elasticity to plate models (WIAS, Dreyer/Sprekels)
- On cell proliferation (WIAS, Wagner/Grothe (University of Basel))

These topics rely on thermodynamic models of large complexity, because they comprise various couplings of different phenomena. Examples are (i) diffusion and mechanical stresses, (ii) liquid flow in magnetic fields with heat conduction. Thus, there arise complex initial-boundary value problems for systems of field equations.

B. Wagner, jointly with R. Klein, J. Sokołowski, and E. Sanchez-Palencia, organized a workshop on *Applications of Asymptotic Analysis* at the Mathematisches Forschungsinstitut Oberwolfach.

In 2006, seven positions in the research group were financed by grants, one by the DFG Priority Program 1095 “Analysis, Modeling, and Simulation of Multiscale Problems”, four by the DFG Research Center MATHEON, dealing with thin film dynamics and crystal growth processes, and one by the DFG Priority Program 1164 “Modeling, Asymptotic Analysis and Numerical Simulation of the Dynamics of Thin Film Nanostructures on Crystal Surfaces”. The seventh position was devoted to a coupling of the flow of heat and matter with time-dependent magnetic fields within the interdisciplinary project *Krist MAG*, which is funded by the Zukunftsfonds Berlin.

Among the numerous collaborations with external partners (i.e., other research institutes, universities, industrial partners) are:

- Theoretical studies on the Becker–Döring system, jointly with the applied analysis group at the Humboldt-Universität zu Berlin, and on the transport of gaseous bubbles in a flowing liquid, jointly with the numerical analysis group at the Otto-von-Guericke-Universität Magdeburg

- Comparison of theoretical simulations with experimental results and their application in crystal growth processes, jointly with the Institute of Crystal Growth in Berlin
- Control and optimization of the dissolution of unwanted precipitates in gallium arsenide (GaAs) wafers, jointly with an industrial producer of semi-insulating GaAs wafers

Selected studies in detail

The following three examples give a more detailed overview on typical problems and their treatment within the research group.

B. Wagner and A. Münch, together with K. Afanasiev and E. Höschele continued a study on flow of thin films in various settings. An important subproblem concerns vertically rotating surfaces of thin plates that pass a liquid bath in order to obtain a uniform coating of the plates.

In a preliminary parameter study, thin Newtonian flows in a PET reactor for small capillary numbers were considered. The study was based on a new mathematical model, a finite element method, and the corresponding FEM code. The evaluation of the results in close collaboration with an industrial partner revealed that non-Newtonian flow and high capillary numbers should also be taken into account. Further discussions lead to the decision to rely now on the FEM code NAVIER, which is developed by the former WIAS member E. Bänsch. To this end, A. Münch, E. Höschele, and K. Afanasiev provided a detailed documentation of that in-house code, and they used the *drag-out problem* for several tests of accuracy, which led to further improvement of the free boundary part of the code NAVIER. This will be important for the accurate treatment of a problem from their industrial partner. On the other hand, B. Wagner and K. Afanasiev tested the applicability, in particular, shear thinning, of various constitutive laws for non-Newtonian liquids. Among these were simple power laws and the CARREAU or ELLIS law. For this purpose, they solved initial-boundary value problems for flows along a tilted plane, [2].

The next example describes the activities of P. Druet, O. Klein, C. Lechner, and J. Sprechels within Krist MAG, which is a joint project of several industrial partners, physicists, engineers, and mathematicians, on the control of unwanted flow patterns in a rotating metallic melt by a changing magnetic field.

From a mathematical viewpoint, the problem is modeled by a coupled initial-boundary value problem for a PDE system consisting of Navier–Stokes equations, the low-frequency approximation of Maxwell's equations, and the heat conduction equation, which is supplemented by a nonlocal radiation boundary condition. For an analytical treatment, P. Druet decomposed the full problem of extreme difficulty into smaller pieces, and he established existence and uniqueness for the stationary as well as for the instationary heat equation, with nonlocal boundary condition and not very regular data. Furthermore, he started to study the existence and uniqueness problem for the stationary incompressible magnetohydrodynamical problem with heat conduction. Simultaneously, O. Klein and C. Lechner carried out numerical calculations relying on the full coupled system. These calculations are based on a combination of two different in-house codes, viz. WIAS-HiTNIHS and NAVIER. These codes were designed as follows: For the growth device, WIAS-HiTNIHS calculates temperature, heat sources, electric currents, magnetic fields, LORENTZ forces, and power

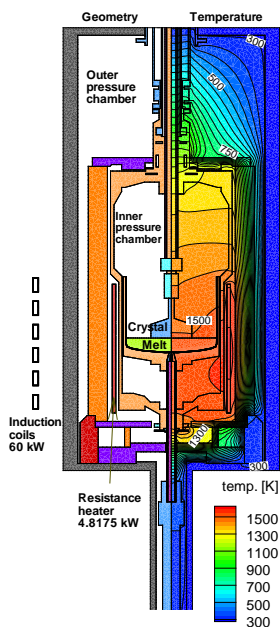


Fig. 1: Vapor pressure controlled Czochralski (VCz) growth arrangement of Institute of Crystal Growth (IKZ), Berlin

supply of the electric coils. The code NAVIER calculates flow fields in the melt, it needs from WIAS-HITNIHS the temperature as initial and boundary data, and the LORENTZ force as an external force. After first tests concerning convergence and accuracy, a study for various control parameters, like speed of rotation, phase shifts of the magnetic field have been carried out to determine their influence on temperature oscillations and the flow field in the melt. Relying on these tests, the physicists were lead to reconstruct the geometric form of the electric coils, [3].

The last example concerns new insights in the dependence of the structure and the geometry of the interface on boundary conditions in phase equilibrium.

W. Dreyer and C. Kraus studied this interplay for the classical sharp interface model with and without boundary contact energy as well as for the corresponding phase field model, the Van der Waals–Cahn–Hilliard model.

In the sharp interface model, a major task was to characterize the structure of the interface for the following configuration which appears in many technological applications, [6].

One prescribes the pressure of the initial system on an arbitrary part of the boundary of the vessel. This part of the boundary may change in time, whereas the other part of the boundary is kept fixed. It has been shown by means of the calculus of variations and methods from differential geometry that the interface has locally a constant mean curvature. A further outstanding result is that in phase equilibrium, the interface can only meet the tight boundary. The corresponding contact angle has also been determined.

Modica showed for the phase field model that in the case of time-independent domains with natural boundary conditions the interface of global minimizers has minimal perimeter. This connection is more involved for Dirichlet boundary conditions.

It turned out that a global minimizer is a minimal solution of an area-type functional consisting of two terms; see [7]. The first term measures the energy with all interior interfaces due to an inner phase transition. The other controls the energy associated with a layer at the boundary. The results were established by γ -convergence, for which several local and global energy estimates were proved. An additional compactness argument ensures that the above results are valid not only for free energies of polynomial growth but also for free energies of logarithmic growth. Moreover, the compactness property generalizes convergence results in the existing literature to the class of free energy functions with logarithmic growth. This is of crucial importance, since an ideal gas or a compressible fluid, for instance, satisfies only the weaker logarithmic growth condition.

References

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- [2] K. AFANASIEV, A. MÜNCH, B. WAGNER, *Thin film dynamics on vertically rotating disks*, WIAS Preprint no. 1074, 2005, to appear in: Appl. Math. Modelling.
- [3] P. DRUET, O. KLEIN, C. LECHNER, *Development of a software for the numerical simulation of VCz growth under the influence of a traveling magnetic field*, to appear in: J. Crystal Growth.
- [4] P. KREJČÍ, E. ROCCA, J. SPREKELS, *A nonlocal phase-field model with nonconstant specific heat*, WIAS Preprint no. 1115, 2006, to appear in: Interfaces Free Bound.

- [5] W. DREYER, M. HERRMANN, A. MIELKE, *Micro-macro transitions in the atomic chain via Whitham's modulation equations*, Nonlinearity, **19** (2006), pp. 471–500.
- [6] W. DREYER, C. KRAUS, *The equilibria of vapour-liquid systems revisited*, WIAS Preprint in preparation.
- [7] C. KRAUS, *The van der Waals–Cahn–Hilliard phase model for fixed domains with Dirichlet boundary conditions*, WIAS Preprint in preparation.

A Facts and Figures

(In the sequel the collaborators of WIAS are underlined.)

- Calls, Awards and Distinctions, Habilitations, Ph.D. Theses
- Grants
- Membership in Editorial Boards
- Conferences, Colloquia, and Workshops
- Membership in Organizing Committees of non-WIAS Meetings
- Publications
- Preprints, Reports
- Talks, Posters, and Contributions to Exhibitions
- Visits to other Institutions
- Academic Teaching
- Weierstrass Postdoctoral Fellowship Program
- Visiting Scientists
- Guest Talks
- Software

A.1 Calls, Awards and Distinctions, Habilitations, Ph.D. Theses

A.1.1 Calls

1. CH. BENDER, Junior professorship, August 10, Technische Universität Braunschweig, Institut für Mathematische Stochastik.
2. B. GENTZ, W2 professorship, April 12, Universität Bielefeld, Fakultät für Mathematik.

A.1.2 Awards and Distinctions

1. A. MIELKE, *member of the Council of the International Society for Interaction of Mathematics and Mechanics (ISIMM)*.
2. J. SPREKELS, *coordinator of the International Mathematical Science Institutes (IMSI)*.
3. ———, *member of the International Scientific Board of the Institute of Mathematics “Simion Stoilow” of the Romanian Academy, Bucharest*.

A.1.3 Ph.D. Theses

1. M. AN DER HEIDEN, *Metastability for Markov chains and in the Hopfield model*, Technische Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. A. Bovier, November 2.
2. M. LICHTNER, *Exponential dichotomy and smooth invariant center manifolds for semilinear hyperbolic systems*, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisors: Dr. habil L. Recke, Prof. Dr. A. Mielke, Prof. Dr. K. Lu, May 30.
3. CH. MEYER, *Optimal control of semilinear elliptic equations with applications to sublimation crystal growth*, Technische Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. F. Tröltzsch, July 19.

A.2 Grants¹

Bundesministerium für Bildung und Forschung (Federal Ministry of Education and Research), Bonn

- **Mathematik für Innovationen in Industrie und Dienstleistungen (Mathematics for innovations in industry and services)**
 “Anwendung eines nichtlokalen Phasenseparationsmodells zur Bildbewertung in der Rheumadiagnostik” (Application of a nonlocal phase separation model to optical diagnosis of rheumatic diseases; in RG 1)
- **Netzwerke Grundlagenforschung erneuerbare Energien und rationelle Energieanwendung** (Networks for basic research in renewable energies and efficient energy use)
 “Numerische Simulation für Direktmethanol-Mikrobrennstoffzellen im Verbund MikroDMFC” (joint project on numerical simulation of direct methanol micro fuel cells in the MikroDMFC network, which is coordinated by the acting head of RG 3)

Deutsche Forschungsgemeinschaft (German Research Foundation), Bonn

- **DFG-Forschungszentrum MATHEON “Mathematik für Schlüsseltechnologien” (DFG Research Center MATHEON “Mathematics for key technologies”)**, Technische Universität Berlin
 A3: “Image and signal processing in medicine and biosciences” (in RG 6)
 A10: “Automatic model reduction for complex dynamical systems” (in RG 6)
 C1: “Coupled systems of reaction-diffusion equations and application to the numerical solution of direct methanol fuel cell (DMFC) problems” (in RG 3)
 C2: “Efficient simulation of flows in semiconductor melts” (in RG 3)
 C7: “Mean-risk optimization of electricity production in liberalized markets” (in RG 4)
 C9: “Numerical simulation and control of sublimation growth of semiconductor bulk single crystals” (in RG 7)
 C10: “Modelling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces” (in RG 7)
 C11: “Modeling and optimization of phase transitions in steel” (in RG 4)
 C14: “Macroscopic models for precipitation in crystalline solids” (in RG 7)
 C17: “Adaptive multigrid methods for local and nonlocal phase-field models of solder alloys” (in RG 7)
 C18: “Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys” (in RG 1)
 C21: “Reduced-order modelling and optimal control of robot guided laser material treatments” (in RG 4)
 D4: “Quantum mechanical and macroscopic models for optoelectronic devices” (in RG 1)
 D8: “Nonlinear dynamical effects in integrated optoelectronic structures” (in RG 2)
 D14: “Nonlocal and nonlinear effects in fiber optics” (in RG 1 and RG 2)
 E1: “Microscopic modelling of complex financial assets” (in RG 5)
 E5: “Statistical and numerical methods in modeling of financial derivatives and valuation of risk” (in RG 6)
 Z1.4: “Innovations in mathematics education for the engineering science” (in RG 4)
- Exzellenzinitiative (German competition for excellence): „Berlin Mathematical School“ (in RG 1, RG 5, and RG 7)

¹The research groups (RG) involved in the respective projects are indicated in brackets.

- Research Training Group GRK 1128, Humboldt-Universität zu Berlin,
“Analysis, Numerics, and Optimization of Multiphase Problems” (in RG 1, RG 3, RG 4, and RG 7)
- Collaborative Research Center (SFB) 555, Humboldt-Universität zu Berlin,
“Komplexe Nichtlineare Prozesse. Analyse — Simulation — Steuerung — Optimierung” (Complex non-linear processes. Analysis — simulation — control — optimization)
B2 “Analytische und numerische Untersuchungen zur raum-zeitlichen Strukturbildung in Halbleiterlasern” (Analytical and numerical investigations on the spatio-temporal formation of structures in semiconductor lasers; in RG 2)
- Collaborative Research Center (SFB) 649, Humboldt-Universität zu Berlin,
“Ökonomisches Risiko” (Economic risk)
B5: “Strukturadaptive Datenanalyse” (Structure-adaptive data analysis; in RG 6)
C4: “Stochastische Optimierung für ökonomische Modelle unter Berücksichtigung von Zeitverzögerungseffekten” (Stochastic optimization for economic models under consideration of time lag effects; in RG 6)
- Priority Program SPP 1095: “Analysis, Modellbildung und Simulation von Mehrskalenproblemen” (Analysis, modeling and simulation of multiscale problems) – Coordinator Program: A. Mielke (in RG 1)
“Elektronische Zustände in Halbleiternanostrukturen und Upscaling auf halbklassische Modelle” (Electronic states in semiconductor nanostructures and upscaling to semi-classical models; in RG 1, RG 3, and RG 4)
“Mikro-Makro-Übergänge mittels Modulationstheorie” (Micro-macro transitions via modulation theory; in RG 7)
“Makroskopische Dynamik in diskreten Gittern” (Macroscopic dynamics in discrete lattices; in RG 1)
- Priority Program SPP 1114: “Mathematische Methoden der Zeitreihenanalyse und digitalen Bildverarbeitung” (Mathematical methods for time series analysis and digital image processing)
“Structure adaptive smoothing procedures with applications in imaging and functional MRI” (in RG 6)
- Priority Program SPP 1135: “Dynamik sedimentärer Systeme unter wechselnden Spannungsregimen am Beispiel des zentraleuropäischen Beckens” (Dynamics of sedimentary systems under varying stress regimes: The example of the Central European Basin)
“Deep reaching fluid-flow in the Central European Basin System” (in RG 3)
- Priority Program SPP 1164: “Nano- und Mikrofluidik: Von der molekularen Bewegung zur kontinuierlichen Strömung” (Nano- & Microfluidics: Bridging the Gap between Molecular Motion and Continuum Flow)
“Mathematical modeling, analysis, numerical simulation of thin films and droplets on rigid and viscoelastic substrates, emphasizing the role of slippage” (in RG 7)
- Priority Program SPP 1180: “Prognose und Beeinflussung der Wechselwirkungen von Strukturen und Prozessen” (Prediction and manipulation of interaction between structure and process)
“Entwicklung eines Prognosetools zur Identifizierung von stabilen Fräsprozessen” (Development of a prognosis tool for the prediction of stable milling processes; in RG 4)
- Priority Program SPP 1204: “Algorithmen zur schnellen, werkstoffgerechten Prozesskettengestaltung und -analyse in der Umformtechnik” (Algorithms for the fast design and analysis of process chains in deformation technology)
“Simulation, Optimierung und Regelung von Gefügebildung und mechanischen Eigenschaften beim Warmwalzen von Mehrphasenstählen” (Simulation and control of phase transitions and mechanical properties during hot-rolling of multiphase steels; in RG 4)

– **Normalverfahren (Individual Grants)**

“Spektralparameterabhängige Randwertprobleme und Hybridmodelle der Halbleitersimulation” (Boundary value problems depending on the spectral parameter and hybrid models in semiconductor simulation; in RG 1)

“Energimodelle für heterogene Halbleiterstrukturen” (Energy models for heterogeneous semiconductor structures; in RG 1)

“Einfluss räumlicher Fluktuationen auf das Gelationsverhalten von Koagulationsprozessen” (Influence of spatial fluctuations on the gelation behavior of coagulation processes; Technische Universität Ilmenau and in RG 5)

“Hydrodynamische Fluktuationen von Verzweigungsmodellen in katalytischen Medien mit unendlicher Erwartung” (Hydrodynamic fluctuations of branching models in catalytic media with infinite expectations; in RG 5)

“Models for phase transition with thermo-mechanical interaction” (in RG 7)

“Mathematical modeling and analysis of spreading polymer films” (in RG 7)

– In 2006, WIAS hosted a scientist with a Heisenberg fellowship (in RG 7).

– A part of the WIAS guest program was supported by DFG grants.

Alexander von Humboldt-Stiftung (Alexander von Humboldt Foundation)

– two scholarship holders (in RG 1 and RG 7), see page 130

Deutscher Akademischer Austauschdienst (German Academic Exchange Service), Bonn

– three scholarship holders (in RG 2, RG 5, and RG 6)

International Projects

– **ESF** (European Science Foundation) Programme “Phase transitions and fluctuation phenomena for random dynamics in spatially extended systems (RDSes)” (in RG 5)

– **EU Research Training Network** “Smart Systems — New materials, adaptive systems and their nonlinearities: Modeling, control and numerical simulation” (in RG 1)

– **GIF** (German-Israeli Foundation for Scientific Research & Development): “Superprocesses and stochastic partial differential equations” (in RG 5)

– **NATO Linkage Grant**: “Stochastic and computational models of transport in porous media” (in RG 6)

– The head of RG 5 is the Coordinator of the International Research Training Group GRK 1339 “Stochastic Models of Complex Systems and their Applications” (DFG/Swiss National Science Foundation).

– The head of RG 5 is also a member of the Bilateral Research Group “Mathematics of random spatial models from physics and biology” (DFG/NWO (Netherlands Organization for Scientific Research)), project: “Equilibrium and ageing in glassy systems”.

Verbundforschungsvorhaben (research network project): “TerabitOptics Berlin”, project B4: “Modellierung und Simulation von Pulsquellen” (Modeling and simulation of pulse sources)

- “Simulation der Pulsausbreitung in nichtlinearen optischen Fasern” (Simulation of pulse propagation in nonlinear optical fibers; in RG 2)
- “Modeling and simulation of mode-locked semiconductor lasers” (in RG 2)

Verbundprojekt (research network project): Krist *MAG* (in RG 7)

Mission-oriented research

- ALSTOM (Switzerland) Ltd., Baden: “Prozesssimulation bei industriellen Gasturbinen” (Process simulation for industrial gas turbines; in RG 3 and RG 6)
- Landesbank Berlin AG (former Bankgesellschaft Berlin): “Implementation of the LIBOR market model, calibration and pricing of derivative products” (in RG 6)
- Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin: “Mathematische Modellierung und Simulation von MOPA-Diodenlasern” (Mathematical modeling and simulation of MOPA diode lasers; in RG 2)
- Fraunhofer-Institut für Nachrichtentechnik Heinrich-Hertz-Institut, Berlin: “diMOLA — Direkt modulierte Laser” (diMOLA — Directly modulated lasers; “Modellierung der dynamischen Eigenschaften von Mehrsektionslasern für deren Einsatz als direkt-modulierte Transmitter-Laser bei Datenraten bis 40 GBs” (Modeling of the dynamic properties of multi-section lasers for their application as directly modulated transmitter laser at data rates up to 40 GBs); in RG 1 and RG 2)
- Freiburger Compound Materials GmbH: “Untersuchung der Evolution einer As-Ausscheidung in GaAs mit einem neu entwickelten Diffusionsmodell zur Erzielung hoher Präzision” (Study of the evolution of a single arsenic precipitate with a newly developed diffusion model that accounts for extremely high precision; in RG 7)
- Rücker GmbH, Weingarten: “Simulations- und Optimierungsaufgaben bei der virtuellen Fabrikplanung” (Simulation and optimal control tasks in virtual production planning in automotive industry; in RG 4)
- Deutsches Elektronen-Synchrotron (German Electron Synchrotron, DESY), Hamburg: “Risikostudie für die Kostenentwicklung des SFEL-Projekts” (Risk study of the development of the costs in the SFEL project; in RG 5)

A.3 Membership in Editorial Boards

1. A. BOVIER, Editorial Board, Electronic Communications in Probability, Institute of Mathematical Statistics (IMS) and Bernoulli Society, Nantes, France.
2. ———, Editorial Board, Electronic Journal of Probability, Institute of Mathematical Statistics (IMS) and Bernoulli Society, Nantes, France.
3. ———, Editorial Board, Markov Processes and Related Fields, Polymat, Russia.
4. K. FLEISCHMANN, Editorial Board, Probability and Mathematical Statistics, Wroclaw University of Technology, Poland.
5. R. HENRION, Editorial Board, International Journal of Management Science and Engineering Management (MSEM), World Academic Press, Liverpool, UK.
6. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
7. P. KREJČÍ, Editor, Applications of Mathematics, Academy of Sciences of the Czech Republic, Prague.
8. P. MATHÉ, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, The Netherlands.
9. ———, Editorial Board, Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.
10. A. MIELKE, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
11. ———, Editor-in-Chief, Journal of Nonlinear Science, Springer Science+Business Media, New York, USA.
12. ———, Editor-in-Chief, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
13. ———, Co-Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
14. ———, Editorial Board, Archive for Rational Mechanics and Analysis, Springer-Verlag, Berlin Heidelberg.
15. ———, Editorial Board, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
16. ———, Editorial Board, SIAM Journal on Mathematical Analysis, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
17. J. POLZEHL, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
18. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.
19. K.K. SABELFELD, Editor, Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.
20. ———, Senior Editor, Mathematics and Computers in Simulation, Elsevier, Amsterdam, The Netherlands.
21. V. SPOKOINY, Editorial Board, Annals of Statistics, IMS, Beachwood, Ohio, USA.
22. ———, Editorial Board, Statistics and Decisions, Oldenbourg Wissenschaftsverlag, München.
23. J. SPREKELS, Editor, Advances in Mathematical Sciences and Applications, Gakkōtoshō, Tokyo, Japan.
24. ———, Editorial Board, Applications of Mathematics, Academy of Sciences of the Czech Republic, Prague.
25. W. WAGNER, Editorial Board, Monte Carlo Methods and Applications, VSP, The Netherlands.

A.4 Conferences, Colloquia, and Workshops

A.4.1 WIAS Conferences, Colloquia, and Workshops

WORKSHOP “NONLINEAR DYNAMICS IN MODELOCKED LASERS AND OPTICAL FIBERS”

Berlin, July 13–14

Organized by: WIAS (RG 2), Humboldt-Universität zu Berlin

Supported by: Technology Foundation Berlin (project “Terabit Optics Berlin”), WIAS

The workshop focused on mathematical, physical, and technological aspects of nonlinear phenomena in semiconductor lasers and optical fibers. The main topics included:

- mode-locking in quantum-well and quantum-dot lasers
- modeling of semiconductor lasers and saturable absorbers
- pulse propagation in nonlinear optical fibers

Being a final workshop related to the applied project “Terabit Optics Berlin”, major attention was paid to an interdisciplinary approach, including the mathematical and physical background as well as technological applications, with a special focus on optical telecommunication technologies. The workshop has been attended by 25 participants from 7 countries, and included 13 invited and contributed talks.

WORKSHOP ON MODELLING AND SIMULATION OF PEM FUEL CELLS

Berlin, September 18–20

Organized by: WIAS (RG 3), Universität Freiburg

Supported by: BMBF, WIAS

This workshop has been organized by J. Fuhrmann and E. Holzbecher of WIAS (RG 3) jointly with M. Oehlberger and B. Haasdonk of Freiburg University (Institute for Applied Mathematics) as an event of the interdisciplinary network “H₂ and Direct Methanol PEM Fuel Cells” supported by the German Federal Ministry of Education and Research within its funding program “Networks in Basic Research for Renewable Energy and Efficient Energy Usage”.

The workshop had 50 international participants, among them several company representatives, and 5 invited speakers. Topics of the workshop were the modeling and simulation of H₂ and methanol fuel cell stacks, with special emphasis on bubble transport. Further topics included the mathematical description of porous transport layers and the three-phase boundary, molecular dynamic simulations of new types of polymer membranes, and the analysis, control, and reduction of complex nonlinear systems.

The workshop strengthened the contacts to the national and international fuel cell community and to industrial partners, and gave significant impulses to the research of the WIAS fuel cell group.

OPENING COLLOQUIUM OF THE INTERNATIONAL RESEARCH TRAINING GROUP (IRTG) GRK 1339 “STOCHASTIC MODELS OF COMPLEX PROCESSES”

Berlin, November 29

Organized by: WIAS (RG 5), Technische Universität Berlin

Supported by: DFG (GRK 1339)

This new research training group of WIAS, Humboldt-Universität zu Berlin, Technische Universität Berlin, Universität Potsdam, Universität Zürich, and ETH Zürich is coordinated by the head of WIAS’s Research Group *Interacting Random Systems* A. Bovier. It will establish an international network for graduate education in applied probability, in which the WIAS will play an important and visible rôle. Nearly 60 participants attended the colloquium, 5 talks were given, followed by a reception at the Swiss Embassy in Berlin.

A.4.2 Non-WIAS Conferences, Colloquia, and Workshops co-organized by WIAS and / or having taken place at WIAS

77TH ANNUAL MEETING OF THE GESELLSCHAFT FÜR ANGEWANDTE MATHEMATIK UND MECHANIK (GAMM), SECTION 8: MULTISCALES AND HOMOGENIZATION

Berlin, March 27–31

Organized by: WIAS (RG 1), Universität Stuttgart

Supported by: DFG, Technische Universität Berlin

Because of the recent strong activities in the field of multiscale modeling, GAMM decided to install an interdisciplinary section on “Multiscales and Homogenization”, which was organized by C. Miehe (Stuttgart) and A. Mielke (WIAS). About 45 talks were held by young researchers as well as by established participants. They concerned the analytical and numerical treatment of material models using Γ -convergence and two-scale approaches (FE² method using periodic Representative Volume Elements (RVE)).

MATHEON WORKSHOP “COMPUTING BY THE NUMBERS: ALGORITHMS, PRECISION, AND COMPLEXITY”

Berlin, July 20–21

Organized by: Humboldt-Universität zu Berlin, WIAS (RG 4)

Supported by: DFG Research Center MATHEON

This international workshop was held in honor of the 60th birthday of Richard Brent. It consisted of four sessions, organized and chaired by leading scientists in their field: Scientific Computing (N. Trefethen, Oxford), Parallel Computing (R. Bisseling, Utrecht), Computational Number Theory (H.J.J. te Riele, Amsterdam), Fast Algorithms (P. Zimmermann, Nancy).

DFG PRIORITY PROGRAM SPP 1180 WORKSHOP “KOPPLUNG VON PROZESS UND STRUKTUR IN MODELLEN DER SPANENDEN FERTIGUNG” (INTERACTION BETWEEN PROCESS AND STRUCTURE IN MODELS OF METAL-CUTTING MANUFACTURING)

Berlin, September 7–8

Organized by: WIAS (RG 4)

The goal of this workshop was to bring together the groups of the DFG Priority Program SPP 1180 “Prediction and Manipulation of Interaction between Structure and Process” working on problems related to metal cutting. The 14 participants discussed different algorithmic coupling approaches and their numerical realization.

WORKSHOP “COMPLEX DYNAMICS AND DELAY EFFECTS IN COUPLED SYSTEMS”

Berlin, September 11–13

Organized by: DFG (SFB 555 “Complex Nonlinear Processes”), WIAS (RG 2), Humboldt-Universität zu Berlin, Technische Universität Berlin, Universität Potsdam

Supported by: DFG (SFB 555 “Complex Nonlinear Processes”)

During this interdisciplinary workshop, physicists and mathematicians discussed new theoretical and experimental results from the field of complex dynamics and coupled systems arising in several areas of applied research. The major topics were:

- coupled systems in optoelectronics and neuroscience
- delay-induced dynamical effects
- synchronization and chaos in coupled systems
- delayed feedback control
- noise in dynamics with delay

The activity in this field of research and the positive response to this interdisciplinary meeting was underlined by the number of 91 registered participants from 17 countries, presenting 39 talks.

INTERNATIONAL CONFERENCE ON MULTIFIELD PROBLEMS (FINAL CONFERENCE OF THE DFG COLLABORATIVE RESEARCH CENTER SFB 404 “MULTIFIELD PROBLEMS IN SOLID AND FLUID MECHANICS”)

Stuttgart, October 4–6

Organized by: Universität Stuttgart, WIAS (RG 1)

Supported by: DFG

The 12 successful years of the SFB 404 were concluded by a conference with 120 participants featuring 12 invited speakers and 10 minisymposia. In particular, all the projects of the SFB presented their recent research results. The topics involved coupling phenomena in continuous and discontinuous media, finite-strain elastoplasticity, fluid-structure interaction, noise propagation, porous media, and multifunctional materials. Special attention was given to the mathematical analysis and the efficient numerical treatment of the models.

CONFERENCE ON MULTISCALE PROBLEMS (FINAL CONFERENCE OF THE DFG PRIORITY PROGRAM SPP 1095 “ANALYSIS, MODELING AND SIMULATION OF MULTISCALE PROBLEMS”)

München, October 9–11

Organized by: Technische Universität München, WIAS (RG 1)

Supported by: DFG (Priority Program SPP 1095 “Analysis, Modeling and Simulation of Multiscale Problems”), Technische Universität München

The conference took place October 9–11 at the Technische Universität München and brought together seven leading scientists from all over the world as well as about 80 German researchers on multiscale problems. The conference marked the official ending of the Priority Program, which started in August 2000. In addition to the seven invited lectures, all the 23 projects within the Priority Program presented and discussed the recent developments within their fields. As a special highlight, the state-of-the-art book “Analysis, Modeling and Simulation of Multiscale Problems” was presented there for the first time in public.

A.5 Membership in Organizing Committees of non-WIAS Meetings

1. U. BANDELOW, member of the Program Committee, *6th International Conference "Numerical Simulation of Optoelectronic Devices" (NUSOD'06)*, Singapore, September 11–14.
2. A. BOVIER, member of the Program Committee, *Frankfurter Stochastik-Tage 2006*, Johann Wolfgang Goethe-Universität Frankfurt, Fachbereich Informatik und Mathematik, March 14–16.
3. ———, member of the Organizing Committee, *BRG Workshop on Random Spatial Models from Physics and Biology (Dutch-German Research Group)*, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, April 4–6.
4. ———, member of the Program Committee, *Workshop on Stochastic Models in Biological Sciences*, Warsaw, Poland, May 29 – June 2.
5. ———, member of the Organizing Committee, *5th Prague Summer School 2006 "Statistical Mathematical Mechanics"*, Charles University in Prague, Center for Theoretical Study and Institute of Theoretical Computer Science, Czech Republic, September 10–23.
6. ———, member of the Organizing Committee, *BRG Workshop on Stochastic Models from Biology and Physics*, Johann Wolfgang Goethe-Universität Frankfurt, October 9–10.
7. W. DREYER, member of the Scientific Committee, *19th International Workshop on "Research in Mechanics of Composites"*, Universität Karlsruhe, Institut für Technische Mechanik, Bad Herrenalb, November 27–29.
8. P. KREJČÍ, organizer of the Special Session "Theory and Applications of Hysteresis Modeling", *6th AIMS International Conference on Dynamical Systems, Differential Equations & Applications*, Université de Poitiers, France, June 25–28.
9. P. MATHÉ, member of the Program Committee, *7th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (MCQMC 2006)*, Universität Ulm, August 14–18.
10. A. MIELKE, co-organizer of the Section "Multiscales and Homogenization", *GAMM Annual Meeting 2006*, Technische Universität Berlin, March 27–31.
11. ———, co-organizer, *International Conference of Multifield Problems (Final Conference of the DFG Collaborative Research Center SFB 404 "Multifield Problems in Solid and Fluid Mechanics")*, Stuttgart, October 4–6.
12. ———, co-organizer, *Conference on Multiscale Problems (Final Conference of the DFG Priority Program SPP 1095 "Analysis, Modeling and Simulation of Multiscale Problems")*, München, October 9–11.
13. ———, member of the Scientific Committee, *European Conference on Smart Systems (Final Meeting of the Research Training Network "New Materials, Adaptive Systems and their Nonlinearities: Modelling, Control and Numerical Simulation")*, Rome, Italy, October 26–28.
14. J. SPREKELS, member of the Scientific Committee, *6th AIMS International Conference on Dynamical Systems, Differential Equations & Applications*, Université de Poitiers, France, June 25–28.
15. B. WAGNER, co-organizer, *Workshop "Applications of Asymptotic Analysis"*, Mathematisches Forschungsinstitut Oberwolfach, June 18–24.
16. M. WOLFRUM, member of the Scientific Committee, *6th Crimean School and Workshops "Nonlinear Dynamics, Chaos and Applications"*, Yalta, Crimea, Ukraine, May 15–26.

A.6 Publications

A.6.1 Monographs

- [1] A. BOVIER, *Statistical Mechanics of Disordered Systems*, vol. 18 of Cambridge Series in Statistical and Probabilistic Mathematics, Cambridge University Press, Cambridge, 2006, xiv+312 pages.
- [2] P. NEITTAANMÄKI, D. TIBA, J. SPREKELS, *Optimization of Elliptic Systems: Theory and Applications*, Springer Monographs in Mathematics, Springer, New York, 2006, xvi+514 pages.

A.6.2 Editorship of Proceedings and Collected Editions

- [1] A. BOVIER, F. DUNLOP, A. VAN ENTER, F. DEN HOLLANDER, J. DALIBARD, eds., *Mathematical Statistical Physics, Proceedings of the 83rd Les Houches Summer School 2005*, Les Houches Summer School Proceedings, Elsevier Science, Amsterdam, 2006, 848 pages.
- [2] A. MIELKE, ed., *Analysis, Modeling and Simulation of Multiscale Problems*, Springer, Berlin, 2006, xviii+697 pages.
- [3] R. HELMIG, A. MIELKE, B. WOHLMUTH, eds., *Multifield Problems in Solid and Fluid Mechanics*, vol. 28 of Lecture Notes in Applied and Computational Mechanics, Springer, Heidelberg, 2006, xi+571 pages.
- [4] P. COLLI, N. KENMOCHI, J. SPREKELS, eds., *Dissipative Phase Transitions*, vol. 71 of Series on Advances in Mathematics for Applied Sciences, World Scientific, Singapore, 2006, xii+300 pages.

Proceedings and Collected Editions (to appear)

- [1] E. BOLTHAUSEN, A. BOVIER, eds., *Spin Glasses*, vol. 1900 of Lecture Notes in Mathematics, Springer, Berlin/Heidelberg.
- [2] K. KUNISCH, G. LEUGERING, J. SPREKELS, F. TRÖLTZSCH, eds., *Control of Coupled Partial Differential Equations*, Internat. Series Numer. Math., Birkhäuser.

A.6.3 Outstanding Contributions to Monographs

- [1] A. BOVIER, *Mean Field Spin Glasses and Neural Networks*, J.-P. FRANÇOISE, G. NABER, T. SCHEUNG, eds., *Encyclopedia of Mathematical Physics*, Elsevier, 2006, pp. 407–412.

A.6.4 Articles in Refereed Journals²

- [1] P.L. EVANS, J.R. KING, A. MÜNCH, *Intermediate-asymptotic structure of a dewetting rim with strong slip*, *Appl. Math. Res. Express*, (2006), pp. 25262/1–25262/25.
- [2] V. PATA, S. ZELIK, *A remark on the weakly damped wave equation*, *Commun. Pure Appl. Anal.*, 5 (2006), pp. 609–614.
- [3] ———, *Smooth attractors for strongly damped wave equations*, *Nonlinearity*, 19 (2006), pp. 1495–1506.

²Articles that have been written by scholarship holders during their stay at WIAS have been listed in front of those written by the collaborators of WIAS.

- [4] B. HÜTTL, H. KAISER, CH. KINDEL, S. FIDORRA, W. REHBEIN, H. STOLPE, G. SAHIN, U. BANDELOW, M. RADZIUNAS, A. VLADIMIROV, H. HEIDRICH, *Experimental investigations on the suppression of Q-switching in monolithic 40 GHz mode-locked semiconductor lasers*, Appl. Phys. Lett., 88 (2006), pp. 221104/1–221104/3.
- [5] U. BANDELOW, M. RADZIUNAS, A. VLADIMIROV, B. HÜTTL, R. KAISER, *Harmonic modelocked semiconductor lasers: Theory, simulations and experiment*, Opt. Quantum Electron., 38 (2006), pp. 495–512.
- [6] D. BELOMESTNY, G. MILSTEIN, *Monte Carlo evaluation of American options using consumption processes*, Int. J. Theor. Appl. Finance, 9 (2006), pp. 455–481.
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- [12] J. DOLATA, H.-J. MUCHA, H.-G. BARTEL, *Uncovering the internal structure of the Roman brick and tile making in Frankfurt-Nied by cluster validation*, in: Proceedings of the 30th Annual Conference of the German Classification Society (GfKI), Springer.
- [13] E. HAIMERL, H.-J. MUCHA, *Comparing the stability of different clustering results of dialect data*, in: Proceedings of the 30th Annual Meeting of Gesellschaft für Klassifikation (GfKI), Springer.
- [14] C. PATZ, A. MIELKE, *Dispersive and long-time behavior of oscillations in lattices*, in: PAMM (Proceedings of Applied Mathematics and Mechanics), Special Issue: GAMM Annual Meeting 2006, Berlin, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim. URL: http://www3.math.tu-berlin.de/gamm_2006.

- [15] J. MARTINS, M.M. MARQUES, A. PETROV, *Mathematical result on the stability of elastic-plastic systems with hardening*, in: Topics on Mathematics for Smart Systems, B. Miara, G. Stavroulakis, V. Valente, eds., World Scientific Publisher.
- [16] T. PEREZ, M. RADZIUNAS, H.-J. WÜNSCHE, C.R. MIRASSO, F. HENNEBERGER, *Chaos synchronization of unidirectionally coupled multisection lasers*, in: Proceedings of the 32nd European Conference on Optical Communication (ECOC 2006).
- [17] F. SCHMID, J. MARTINS, N. REBROVA, *New results on the stability of quasi-static paths of a single particle system with Coulomb friction and persistent contact*, in: Topics on Mathematics for Smart Systems, B. Miara, G. Stavroulakis, V. Valente, eds., World Scientific Publisher.
- [18] A. SEGATTI, *Global attractors for the quasistationary phase field model: A gradient flow approach*, in: Free Boundary Problems. Theory and Applications, I.N. Figueiredo, J.F. Rodrigues, L. Santos, eds., Internat. Ser. Numer. Math., Birkhäuser.
- [19] A. STEINBRECHER, *Numerical simulation of multibody systems via Runge–Kutta methods*, in: PAMM (Proceedings of Applied Mathematics and Mechanics), Special Issue: GAMM Annual Meeting 2006, Berlin, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim. URL: http://www3.math.tu-berlin.de/gamm_2006.
- [20] A. TIMOFTE, *On modeling, analytical study and homogenization for smart materials*, in: Topics on Mathematics for Smart Systems, B. Miara, G. Stavroulakis, V. Valente, eds., World Scientific Publisher.
- [21] A. TIMOFTE, A. MIELKE, *Two-scale homogenization for rate-independent systems*, in: PAMM (Proceedings of Applied Mathematics and Mechanics), Special Issue: GAMM Annual Meeting 2006, Berlin, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim. URL: http://www3.math.tu-berlin.de/gamm_2006.

A.7 Preprints, Reports

A.7.1 WIAS Preprints Series³

- [1] M. ELEUTERI, *Well posedness results for a class of partial differential equations with hysteresis arising in electromagnetism*, Preprint no. 1163, WIAS, Berlin, 2006.
- [2] K. EPPLER, *A shape calculus analysis for tracking type formulations in electrical impedance tomography*, Preprint no. 1116, WIAS, Berlin, 2006.
- [3] K. EPPLER, H. HARBRECHT, M. MOMMER, *A new fictitious domain method in shape optimization*, Preprint no. 1117, WIAS, Berlin, 2006.
- [4] P.L. EVANS, J.R. KING, A. MÜNCH, *Intermediate-asymptotic structure of a dewetting rim with strong slip*, Preprint no. 1183, WIAS, Berlin, 2006.
- [5] S. GATTI, A. MIRANVILLE, V. PATA, S. ZELIK, *Attractors for semilinear equations of viscoelasticity with very low dissipation*, Preprint no. 1139, WIAS, Berlin, 2006.
- [6] C. LEFTER, *Feedback stabilization of magnetohydrodynamic equations*, Preprint no. 1144, WIAS, Berlin, 2006.
- [7] V. PATA, S. ZELIK, *Attractors and their regularity for 2-D wave equations with nonlinear damping*, Preprint no. 1140, WIAS, Berlin, 2006.
- [8] ———, *Global and exponential attractors for 3-D wave equations with displacement dependent damping*, Preprint no. 1138, WIAS, Berlin, 2006.
- [9] ———, *Global attractors for semigroups of closed operators*, Preprint no. 1141, WIAS, Berlin, 2006.
- [10] ———, *A remark on the weakly damped wave equation*, Preprint no. 1142, WIAS, Berlin, 2006.
- [11] ———, *Smooth attractors for strongly damped wave equations*, Preprint no. 1137, WIAS, Berlin, 2006.
- [12] B. SCHMALFUSS, K.R. SCHNEIDER, *Invariant manifolds for random dynamical systems with slow and fast variables*, Preprint no. 1157, WIAS, Berlin, 2006.
- [13] B. HÜTTL, R. KAISER, CH. KINDEL, S. FIDORRA, W. REHBEIN, H. STOLPE, G. SAHIN, U. BANDELOW, M. RADZIUNAS, A. VLADIMIROV, H. HEIDRICH, *Experimental investigations on the suppression of Q-switching in monolithic 40 GHz mode-locked semiconductor lasers*, Preprint no. 1112, WIAS, Berlin, 2006.
- [14] D. BELOMESTNY, P. GAPEEV, *An iteration procedure for solving integral equations related to the American put options*, Preprint no. 1105, WIAS, Berlin, 2006.
- [15] D. BELOMESTNY, CH. BENDER, J.G. SCHOENMAKERS, *True upper bounds for Bermudan products via non-nested Monte Carlo*, Preprint no. 1186, WIAS, Berlin, 2006.
- [16] D. BELOMESTNY, J.G.M. SCHOENMAKERS, *A jump-diffusion Libor model and its robust calibration*, Preprint no. 1113, WIAS, Berlin, 2006.
- [17] D. BELOMESTNY, G.N. MILSTEIN, V. SPOKOINY, *Regression methods in pricing American and Bermudan options using consumption processes*, Preprint no. 1145, WIAS, Berlin, 2006.
- [18] CH. BENDER, T. SOTTINEN, E. VALKEILA, *No-arbitrage pricing beyond semimartingales*, Preprint no. 1110, WIAS, Berlin, 2006.
- [19] CH. BENDER, J. ZHANG, *Time discretization and Markovian iteration for coupled FBSDEs*, Preprint no. 1160, WIAS, Berlin, 2006.

³Preprints that have been written by guests during their stay at WIAS have been listed in front of those written by the collaborators of WIAS.

- [20] M. BIRKNER, A. DEPPERSCHMIDT, *Survival and complete convergence for a spatial branching system with local regulation*, Preprint no. 1147, WIAS, Berlin, 2006.
- [21] A. BOVIER, J. ČERNÝ, *Hydrodynamic limit for the $A + B \rightarrow \emptyset$ model*, Preprint no. 1114, WIAS, Berlin, 2006.
- [22] N. CHAMPAGNAT, A. LAMBERT, *Discrete logistic branching populations and the canonical diffusion of adaptive dynamics*, Preprint no. 1095, WIAS, Berlin, 2006.
- [23] N. CHAMPAGNAT, S. MÉLÉARD, *Invasion and adaptive evolution for individual-based spatially structured populations*, Preprint no. 1118, WIAS, Berlin, 2006.
- [24] A. DEMIRCAN, U. BANDELOW, *Analysis of the interplay between soliton fission and modulation instability in supercontinuum generation*, Preprint no. 1102, WIAS, Berlin, 2006.
- [25] ———, *Limit for pulse compression by pulse splitting*, Preprint no. 1153, WIAS, Berlin, 2006.
- [26] A. DEMIRCAN, M. KROH, U. BANDELOW, B. HÜTTL, H.-G. WEBER, *Compression limit by third-order dispersion in the normal dispersion regime*, Preprint no. 1108, WIAS, Berlin, 2006.
- [27] TH. BÖHME, W. DREYER, W.H. MÜLLER, *Determination of stiffness and higher gradient coefficients by means of the embedded atom method: An approach for binary alloys*, Preprint no. 1131, WIAS, Berlin, 2006.
- [28] W. DREYER, CH. KRAUS, *The sharp interface limit of the van der Waals–Cahn–Hilliard phase model for fixed and time dependent domains*, Preprint no. 1103, WIAS, Berlin, 2006.
- [29] W. DREYER, M. HERRMANN, J.D.M. RADEMACHER, *Wave trains, solitons and modulation theory in FPU chains*, Preprint no. 1132, WIAS, Berlin, 2006.
- [30] J. ELSCHNER, J. REHBERG, G. SCHMIDT, *Optimal regularity for elliptic transmission problems including C^1 interfaces*, Preprint no. 1094, WIAS, Berlin, 2006.
- [31] K. FLEISCHMANN, C. MUELLER, P. VOGT, *On the large scale behavior of super-Brownian motion in three dimensions with a single point source*, Preprint no. 1154, WIAS, Berlin, 2006.
- [32] K. FLEISCHMANN, V. WACHTEL, *Large deviations for sums defined on a Galton–Watson process*, Preprint no. 1135, WIAS, Berlin, 2006.
- [33] K. FLEISCHMANN, P. MÖRTERS, V. WACHTEL, *Moderate deviations for random walk in random scenery*, Preprint no. 1167, WIAS, Berlin, 2006.
- [34] K. FLEISCHMANN, V.A. VATUTIN, V. WACHTEL, *Critical Galton–Watson processes: The maximum of total progenies within a large window*, Preprint no. 1091, WIAS, Berlin, 2006.
- [35] P. GAPEEV, *Discounted optimal stopping for maxima of some jump-diffusion processes*, Preprint no. 1161, WIAS, Berlin, 2006.
- [36] ———, *Multiple disorder problems for Wiener and compound Poisson processes with exponential jumps*, Preprint no. 1174, WIAS, Berlin, 2006.
- [37] P. GAPEEV, *Nonadditive disorder problems for some diffusion processes*, Preprint no. 1181, WIAS, Berlin, 2006.
- [38] P. GAPEEV, *On maximal inequalities for some jump processes*, Preprint no. 1162, WIAS, Berlin, 2006.
- [39] ———, *Sequential testing problems for some diffusion processes*, Preprint no. 1178, WIAS, Berlin, 2006.
- [40] D. DAOUD, J. GEISER, *Fractional-splitting and domain-decomposition methods for parabolic problems and applications*, Preprint no. 1096, WIAS, Berlin, 2006.
- [41] J. GIANNOULIS, M. HERRMANN, A. MIELKE, *Continuum descriptions for the dynamics in discrete lattices: Derivation and justification*, Preprint no. 1126, WIAS, Berlin, 2006.
- [42] A. GLITZKY, *Energy estimates for electro-reaction-diffusion systems with partly fast kinetics*, Preprint no. 1158, WIAS, Berlin, 2006.

- [43] A. GLITZKY, R. HÜNLICH, *Resolvent estimates in $W^{-1,p}$ related to strongly coupled linear parabolic systems with coupled nonsmooth capacities*, Preprint no. 1086, WIAS, Berlin, 2006.
- [44] ———, *Stationary solutions to an energy model for semiconductor devices where the equations are defined on different domains*, Preprint no. 1173, WIAS, Berlin, 2006.
- [45] R. HENRION, *Structural properties of linear probabilistic constraints*, Preprint no. 1089, WIAS, Berlin, 2006.
- [46] R. HENRION, CH. KÜCHLER, W. RÖMISCH, *Scenario reduction in stochastic programming with respect to discrepancy distances*, Preprint no. 1185, WIAS, Berlin, 2006.
- [47] R. HENRION, J. OUTRATA, *On calculating the normal cone to a finite union of convex polyhedra*, Preprint no. 1146, WIAS, Berlin, 2006.
- [48] D. HÖMBERG, M. YAMAMOTO, *Exact controllability on a curve for a semilinear parabolic equation*, Preprint no. 1097, WIAS, Berlin, 2006.
- [49] H.-CHR. KAISER, H. NEIDHARDT, J. REHBERG, *Classical solutions of drift-diffusion equations for semiconductor devices: The 2D case*, Preprint no. 1189, WIAS, Berlin, 2006.
- [50] D. KNEES, A.-M. SÄNDIG, *Regularity of elastic fields in composites*, Preprint no. 1129, WIAS, Berlin, 2006.
- [51] D. KNEES, A. MIELKE, *Energy release rate for cracks in finite-strain elasticity*, Preprint no. 1100, WIAS, Berlin, 2006.
- [52] TH. KOPRUCKI, H.-CHR. KAISER, J. FUHRMANN, *Electronic states in semiconductor nanostructures and up-scaling to semi-classical models*, Preprint no. 1133, WIAS, Berlin, 2006.
- [53] CH. KRAUS, *Maximal convergence theorems for functions of squared modulus holomorphic type in R^2 and various applications*, Preprint no. 1175, WIAS, Berlin, 2006.
- [54] ———, *A solution of Braess' approximation problem on powers of the distance function*, Preprint no. 1171, WIAS, Berlin, 2006.
- [55] M. ELEUTERI, P. KREJČÍ, *Asymptotic behavior of a Neumann parabolic problem with hysteresis*, Preprint no. 1109, WIAS, Berlin, 2006.
- [56] P. KREJČÍ, J. SPREKELS, *The von Mises model for one-dimensional elastoplastic beams and Prandtl-Ishlinskii hysteresis operators*, Preprint no. 1143, WIAS, Berlin, 2006.
- [57] P. KREJČÍ, E. ROCCA, J. SPREKELS, *A nonlocal phase-field model with nonconstant specific heat*, Preprint no. 1115, WIAS, Berlin, 2006.
- [58] M. LICHTNER, *Principle of linearized stability and smooth center manifold theorem for semilinear hyperbolic systems*, Preprint no. 1155, WIAS, Berlin, 2006.
- [59] ———, *Spectral mapping theorem for linear hyperbolic systems*, Preprint no. 1150, WIAS, Berlin, 2006.
- [60] E. BURMAN, A. LINKE, *Stabilized finite element schemes for incompressible flow using Scott–Vogelius elements*, Preprint no. 1165, WIAS, Berlin, 2006.
- [61] P. MATHÉ, B. HOFMANN, *Analysis of profile functions for general linear regularization methods*, Preprint no. 1107, WIAS, Berlin, 2006.
- [62] P. MATHÉ, E. NOVAK, *Simple Monte Carlo and the Metropolis algorithm*, Preprint no. 1182, WIAS, Berlin, 2006.
- [63] P. MATHÉ, U. TAUTENHAHN, *Interpolation in variable Hilbert scales with application to inverse problems*, Preprint no. 1148, WIAS, Berlin, 2006.
- [64] CH. MEYER, *Error estimates for the finite-element approximation of an elliptic control problem with pointwise state and control constraints*, Preprint no. 1159, WIAS, Berlin, 2006.
- [65] M. HINZE, CH. MEYER, *Numerical analysis of Lavrentiev-regularized state constrained elliptic control problems*, Preprint no. 1168, WIAS, Berlin, 2006.

- [66] A. MIELKE, *A mathematical framework for standard generalized materials in the rate-independent case*, Preprint no. 1123, WIAS, Berlin, 2006.
- [67] ———, *A model for temperature-induced phase transformations in finite-strain elasticity*, Preprint no. 1184, WIAS, Berlin, 2006.
- [68] F. AURICCHIO, A. MIELKE, U. STEFANELLI, *A rate-independent model for the isothermal quasi-static evolution of shape-memory materials*, Preprint no. 1170, WIAS, Berlin, 2006.
- [69] A. MIELKE, M. ORTIZ, *A class of minimum principles for characterizing the trajectories and the relaxation of dissipative systems*, Preprint no. 1136, WIAS, Berlin, 2006.
- [70] A. MIELKE, T. ROUBÍČEK, *Numerical approaches to rate-independent processes and applications in inelasticity*, Preprint no. 1169, WIAS, Berlin, 2006.
- [71] A. MIELKE, T. ROUBÍČEK, U. STEFANELLI, *Γ -limits and relaxations for rate-independent evolutionary problems*, Preprint no. 1156, WIAS, Berlin, 2006.
- [72] E. GÜRSER, A. MAINIK, CH. MIEHE, A. MIELKE, *Analytical and numerical methods for finite-strain elastoplasticity*, Preprint no. 1127, WIAS, Berlin, 2006.
- [73] A. MIELKE, A. TIMOFTE, *Two-scale homogenization for evolutionary variational inequalities via the energetic formulation*, Preprint no. 1172, WIAS, Berlin, 2006.
- [74] S. ZELIK, A. MIELKE, *Multi-pulse evolution and space-time chaos in dissipative systems*, Preprint no. 1093, WIAS, Berlin, 2006.
- [75] J. BEHRNDT, M. MALAMUD, H. NEIDHARDT, *Scattering theory for open quantum systems*, Preprint no. 1179, WIAS, Berlin, 2006.
- [76] J. BEHRNDT, M.M. MALAMUD, H. NEIDHARDT, *Scattering matrices and Weyl functions*, Preprint no. 1121, WIAS, Berlin, 2006.
- [77] M. PIETRZYK, I. KANATTSIKOV, U. BANDELOW, *On the propagation of vector ultra-short pulses*, Preprint no. 1134, WIAS, Berlin, 2006.
- [78] J. POLZEHL, K. TABELOW, *Adaptive smoothing of digital images: The R package adimpro*, Preprint no. 1177, WIAS, Berlin, 2006.
- [79] M. RADZIUNAS, A. GLITZKY, U. BANDELOW, M. WOLFRUM, U. TROPPEZ, J. KREISSEL, W. REHBEIN, *Improving the modulation bandwidth in semiconductor lasers by passive feedback*, Preprint no. 1149, WIAS, Berlin, 2006.
- [80] M. RADZIUNAS, H.-J. WÜNSCHE, B. KRAUSKOPF, M. WOLFRUM, *External cavity modes in Lang-Kobayashi and traveling wave models*, Preprint no. 1111, WIAS, Berlin, 2006.
- [81] H. GROSS, A. RATHSFELD, *Sensitivity analysis for indirect measurement in scatterometry and the reconstruction of periodic grating structures*, Preprint no. 1164, WIAS, Berlin, 2006.
- [82] H. GROSS, R. MODEL, M. BÄR, M. WURM, B. BODERMANN, A. RATHSFELD, *Mathematical modelling of indirect measurements in periodic diffractive optics and scatterometry*, Preprint no. 1099, WIAS, Berlin, 2006.
- [83] A. RATHSFELD, G. SCHMIDT, B.H. KLEEMANN, *On a fast integral equation method for diffraction gratings*, Preprint no. 1090, WIAS, Berlin, 2006.
- [84] M. HIEBER, J. REHBERG, *Quasilinear parabolic systems with mixed boundary conditions*, Preprint no. 1124, WIAS, Berlin, 2006.
- [85] O. ROTT, D. HÖMBERG, C. MENSE, *A comparison of analytical cutting force models*, Preprint no. 1151, WIAS, Berlin, 2006.
- [86] K.K. SABELFELD, I. SHALIMOVA, A. LEVYKIN, *Random walk on fixed spheres for Laplace and Lamé equations*, Preprint no. 1106, WIAS, Berlin, 2006.
- [87] F. SCHMID, J.A.C. MARTINS, N. REBROVA, *New results on the stability of quasi-static paths of a single particle system with Coulomb friction and persistent contact*, Preprint no. 1190, WIAS, Berlin, 2006.

- [88] F. SCHMID, A. MIELKE, *Existence results for a contact problem with varying friction coefficient and nonlinear forces*, Preprint no. 1188, WIAS, Berlin, 2006.
- [89] V. MAZ'YA, G. SCHMIDT, *Potentials of Gaussians and approximate wavelets*, Preprint no. 1104, WIAS, Berlin, 2006.
- [90] D. SPIVAKOVSKAYA, A. HEEMINK, J.G.M. SCHOENMAKERS, *Two-particle models for the estimation of the mean and standard deviation of concentrations in coastal waters*, Preprint no. 1088, WIAS, Berlin, 2006.
- [91] G.N. MILSTEIN, J.G.M. SCHOENMAKERS, V. SPOKOINY, *Forward and reverse representations for Markov chains*, Preprint no. 1125, WIAS, Berlin, 2006.
- [92] G. SCHIMPERNA, A. SEGATTI, *Attractors for the semiflow associated with a class of doubly nonlinear parabolic equations*, Preprint no. 1194, WIAS, Berlin, 2006.
- [93] H. SI, *Adaptive tetrahedral mesh generation by constrained Delaunay refinement*, Preprint no. 1176, WIAS, Berlin, 2006.
- [94] G. BLANCHARD, M. KAWANABE, M. SUGIYAMA, V. SPOKOINY, K.-R. MÜLLER, *In search of non-Gaussian components of a high-dimensional distribution*, Preprint no. 1092, WIAS, Berlin, 2006.
- [95] V. KATKOVNIK, V. SPOKOINY, *Spatially adaptive estimation via fitted local likelihood techniques*, Preprint no. 1166, WIAS, Berlin, 2006.
- [96] C. LEFTER, J. SPREKELS, *Optimal boundary control of a phase field system modeling nonisothermal phase transitions*, Preprint no. 1187, WIAS, Berlin, 2006.
- [97] H. STEPHAN, *Modeling of drift-diffusion systems*, Preprint no. 1120, WIAS, Berlin, 2006.
- [98] K. TABELOW, J. POLZEHL, A.M. ULUČ, J.P. DYKE, R. WATTS, L.A. HEIER, H.U. VOSS, *Accurate localization of brain activity in presurgical fMRI by structure adaptive smoothing*, Preprint no. 1119, WIAS, Berlin, 2006.
- [99] A. TIMOFTE, *On modeling, analytical study and homogenization for smart materials*, Preprint no. 1180, WIAS, Berlin, 2006.
- [100] D. TURAEV, A. VLADIMIROV, S. ZELIK, *Chaotic bound state of localized structures in the complex Ginzburg–Landau equation*, Preprint no. 1152, WIAS, Berlin, 2006.
- [101] E. VIKTOROV, P. MANDEL, A. VLADIMIROV, U. BANDELOW, *A model for mode-locking in quantum dot lasers*, Preprint no. 1098, WIAS, Berlin, 2006.
- [102] R. FETZER, M. RAUSCHER, A. MÜNCH, B. WAGNER, K. JACOBS, *Slip-controlled thin film dynamics*, Preprint no. 1191, WIAS, Berlin, 2006.
- [103] A. MÜNCH, B. WAGNER, M. RAUSCHER, R. BLOSSEY, *A thin film model for corotational Jeffreys fluids under strong slip*, Preprint no. 1193, WIAS, Berlin, 2006.
- [104] R. BLOSSEY, A. MÜNCH, M. RAUSCHER, B. WAGNER, *Slip vs. viscoelasticity in dewetting thin films*, Preprint no. 1192, WIAS, Berlin, 2006.
- [105] W. WAGNER, *Post-gelation behavior of a spatial coagulation model*, Preprint no. 1128, WIAS, Berlin, 2006.
- [106] S. RJASANOW, W. WAGNER, *Time splitting error in DSMC schemes for the inelastic Boltzmann equation*, Preprint no. 1087, WIAS, Berlin, 2006.
- [107] M. WOLFRUM, S. YANCHUK, *Oscillatory instability in systems with delay*, Preprint no. 1101, WIAS, Berlin, 2006.
- [108] A. POLITI, F. GINELLI, S. YANCHUK, Y. MAISTRENKO, *From synchronization to Lyapunov exponents and back*, Preprint no. 1130, WIAS, Berlin, 2006.
- [109] S. YANCHUK, M. WOLFRUM, P. HÖVEL, E. SCHÖLL, *Control of unstable steady states by strongly delayed feedback*, Preprint no. 1122, WIAS, Berlin, 2006.

A.7.2 WIAS Technical Reports Series

- [1] J. POLZEHL, K. TABELOW, *Analysing fMRI experiments with the fmri package in R. Version 1.0 — A users guide*, WIAS Report no. 10, WIAS, Berlin, 2006.

A.7.3 Preprints/Reports in other Institutions

- [1] P. MATHÉ, B. HOFMANN, *Direct and inverse results in variable Hilbert scales*, Preprint no. 27, Technische Universität Chemnitz, Fakultät für Mathematik, 2006.
- [2] R. ROSSI, A. SEGATTI, U. STEFANELLI, *Attractors for gradient flows of non convex functionals and applications*, Preprint no. 5-PV, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, 2006.

A.8 Talks, Posters, and Contributions to Exhibitions

A.8.1 Scientific Talks (Invited)

1. U. BANDELOW, *Modeling and simulation of optoelectronic devices*, Kick-off Workshop “Materials in New Light”, Humboldt-Universität zu Berlin, Institut für Physik, Berlin, January 6.
2. ———, *Simulation and analysis of spatio-temporal effects in complex laser structures*, Kick-off Workshop “Materials in New Light”, Humboldt-Universität zu Berlin, Institut für Physik, Berlin, January 6.
3. ———, *Modellierung und Simulation optoelektronischer Bauelemente*, Berliner Industriegespräche, Deutsche Physikalische Gesellschaft, Magnus-Haus, Berlin, September 6.
4. A. BARANOWSKI, *Stochastische Analyse von Sonnenflecken und die resultierende nicht-lineare Vorhersage ihrer Zyklen*, Dresdner Mathematisches Seminar, Technische Universität Dresden, Fakultät Mathematik und Naturwissenschaften, December 6.
5. D. BELOMESTNY, *Spectral calibration of exponential Lévy models*, Universität Bonn, Institut für Angewandte Mathematik, Collaborative Research Center SFB 611 “Singular Phenomena and Scaling in Mathematical Models”, January 19.
6. ———, *Spatial aggregation of local likelihood estimates with application to classification*, Universität Heidelberg, Institut für Angewandte Mathematik, February 9.
7. CH. BENDER, *Mixed fractional Brownian motion in finance*, Martin-Luther-Universität Halle-Wittenberg, Institut für Optimierung und Stochastik, January 30.
8. ———, *No-arbitrage pricing beyond semimartingales*, Helsinki University of Technology, Institute of Mathematics, Finland, March 8.
9. ———, *Arbitrage with fractional Brownian motion?*, Workshop on Modern Stochastics: Theory and Applications, June 18–24, Kiev, Ukraine, June 21.
10. ———, *Time discretization and Markovian iteration for coupled FBSDEs*, Workshop on Securitization of Weather and Climate Risk, August 31 – September 2, Humboldt-Universität zu Berlin, August 31.
11. M. BIRKNER, *Große Abweichungen für eine bedingte Verteilung und Anwendungen auf räumliche Systeme mit zufälliger Umgebung*, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, January 24.
12. ———, *Large deviations for a conditional distribution and potential applications to directed polymers in random environment*, Séminaire de Probabilités et Statistique, Université de Provence, Laboratoire d’Analyse, Topologie, Probabilités, Marseille, France, February 17.
13. ———, *Likelihood-based inference for Λ -coalescents under the infinitely-many-sites model*, Workshop “Koaleszententheorie”, Universität Köln, Institut für Genetik, October 2.
14. ———, *Likelihood-based inference for Λ -coalescents under the infinitely-many-sites model*, BRG Workshop on Stochastic Models from Biology and Physics, October 9–10, Johann Wolfgang Goethe-Universität Frankfurt, October 9.
15. A. BOVIER, *Towards a spectral approach to ageing*, Workshop on Relaxational Dynamics of Macroscopic Systems, January 9–13, University of Cambridge, Isaac Newton Institute for Mathematical Sciences, UK, January 11.
16. ———, *A short course in mean field spin glasses*, 2 talks, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, February 2.
17. ———, *Metastability: A potential theoretic approach*, Università degli Studi di Firenze, Dipartimento di Fisica, Italy, June 7.

18. ———, *Metastability: A potential theoretic approach*, International Congress of Mathematicians, August 22–30, Madrid, Spain, August 25.
19. ———, *Lectures on metastability*, 3 talks, 5th Prague Summer School 2006 “Statistical Mathematical Mechanics”, Charles University, Center for Theoretical Study and Institute of Theoretical Computer Science, Prague, Czech Republic, September 10–23.
20. ———, *Rigorous perspectives on spin glasses*, Workshop on Microscopic Approaches to Elastic and Surface Tension Functionals, October 16–26, Università degli Studi di Roma “Tor Vergata”, Dipartimento di Matematica, Italy, October 25.
21. ———, *Recent progress on the spin glass problem*, Workshop “Algorithms for the SAT problem”, October 27–29, Humboldt-Universität zu Berlin, October 29.
22. A. BRADJI, *An approach to improve convergence order in finite volume methods and its application in finite element methods*, Instituto Superior Técnico, Lisboa, Portugal, July 14.
23. N. CHAMPAGNAT, *Invasion and adaptive evolution for individual-based spatially structured populations*, March 25–30, University of Edinburgh, School of Mathematics, UK, March 27.
24. ———, *Robustness in discrete logistic branching populations and the canonical diffusion of adaptive dynamics*, BRG Workshop on Random Spatial Models from Physics and Biology, April 4–6, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, April 5.
25. ———, *Une interprétation microscopique d'un processus stochastique d'évolution par sauts en dynamiques adaptatives et conséquences biologiques*, Séminaires de Mathématiques, Université Claude Bernard Lyon 1, Institut Camille Jordan, France, April 13.
26. ———, *Le phénomène de branchement évolutif: une interprétation microscopique en dynamiques adaptatives*, Université de Nice Sophia Antipolis, France, May 4.
27. W. DREYER, *Precipitation in liquid/vapor and liquid/solid systems*, Seminar Dipartimento di Matematica, Università degli Studi di Trento, Italy, February 7.
28. ———, *Evolution of intermetallic phases in solder bonds*, EuroSimE 2006, April 23–26, Como, Italy, April 26.
29. ———, *Review and new results on nucleation problems*, Polish-German Workshop “Modeling Structure Formation”, Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Poland, September 8.
30. ———, *Thermodynamics and kinetic theory of nucleation and the evolution of liquid precipitation in gallium arsenide wafer*, 5th International Workshop on Modeling in Crystal Growth (IWMCG-5), September 10–13, Bamberg, September 12.
31. ———, *Equilibria of bubbles in a ternary liquid*, Workshop on Modelling and Simulation of PEM Fuel Cells, September 18–20, WIAS, Berlin, September 18.
32. ———, *On the role of non-convex energy functions in thermodynamics*, 19th International Workshop on “Research in Mechanics of Composites”, November 27–29, Universität Karlsruhe, Institut für Technische Mechanik, Bad Herrenalb, November 28.
33. ———, *Bizarre, erheiternde und ernste Begebenheiten zur Entdeckung der beiden Hauptsätze der Thermodynamik*, Deutsche Gesellschaft für Zerstörungsfreie Prüfung e.V., Arbeitskreis Zwickau-Chemnitz, Westsächsische Hochschule Zwickau (FH), December 5.
34. ———, *Thermodynamic properties of the atomic chain for various micro-macro transitions*, Nonlinear Dynamics of Acoustic Modes in Finite Lattices: Localization, Equipartition, Transport, December 6–8, Max-Planck-Institut für Physik komplexer Systeme, Dresden, December 6.
35. W. DREYER, W.H. MÜLLER, *Die sieben Todsünden in der Wissenschaft*, DVM-Tag 2006, Deutscher Verband für Materialforschung und -prüfung e.V., May 9–11, Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, May 10.

36. F. DUDERSTADT, *Ein Becker-Döring-Modell zur Entstehung von Ausscheidungen in GaAs*, 7. Kinetikseminar der DGKK, February 14–15, Max-Planck-Institut für Mikrostrukturphysik, Halle, February 14.
37. ———, *Thermodynamik, kinetische Keimbildungstheorie und Evolution von flüssigen Ausscheidungen in Gallium-Arsenid-Wafern*, Wissenschaftsseminar zur Präzipitatbildung, Freiburger Compound Materials GmbH sowie Institut für Kristallzüchtung, Berlin, December 4.
38. J. ELSCHNER, *Variational approach to scattering by unbounded surfaces*, 12th Conference on Mathematics of Finite Elements and Applications (MAFELAP 2006), June 13–16, Brunel University, Uxbridge, UK, June 15.
39. ———, *Inverse problems for diffraction gratings*, Waves Meeting, September 21–23, University of Reading, UK, September 22.
40. ———, *Variational approach to scattering by unbounded surfaces*, Autumn School “Analysis of Maxwell’s Equations” (Research Training Group GRK 1294 “Analysis, Simulation and Design of Nanotechnological Processes”), October 17–19, Universität Karlsruhe, October 18.
41. M.H. FARSHBAF SHAKER, *On a nonlocal viscose phase separation model*, 6th AIMS International Conference on Dynamical Systems, Differential Equations & Applications, June 25–28, Université de Poitiers, France, June 28.
42. ———, *Ein nichtlokales Phasenseparationsmodell*, Universität Bonn, Institut für Angewandte Mathematik, December 8.
43. M. FISCHER, *Higher-order approximation of infinite horizon control problems for continuous time stochastic systems with delay*, Università di Roma “La Sapienza”, Dipartimento di Matematica, Italy, March 6.
44. P. GAPEEV, *About construction of jump analogues of diffusion processes*, Seminar on Stochastics, Helsinki University of Technology, Institute of Mathematics, Finland, October 9.
45. B. GENTZ, *Dansgaard-Oeschger events, residence times, and stochastic resonance*, Westfälische Wilhelms-Universität Münster, Mathematisch-Naturwissenschaftliche Fakultät, April 20.
46. ———, *Concentration of sample paths in stochastic slow-fast systems*, 6th AIMS International Conference on Dynamical Systems, Differential Equations & Applications, June 25–28, Université de Poitiers, France, June 27.
47. ———, *Metastability in irreversible diffusion processes and stochastic resonance*, SIAM Annual Meeting, July 10–14, Boston, USA, July 12.
48. ———, *Noise-induced phenomena in slow-fast dynamical systems*, SIAM Annual Meeting, July 10–14, Boston, USA, July 12.
49. J. GIANNOULIS, *Three wave interaction in discrete lattices*, 5th GAMM Seminar on Microstructures, January 13–14, Universität Duisburg-Essen, Essen, January 14.
50. ———, *Three-wave interaction for discrete lattices*, Technische Universität München, Zentrum Mathematik, February 6.
51. A. GLITZKY, *Energy estimates for electro-reaction-diffusion systems with partly fast kinetics*, 6th AIMS International Conference on Dynamical Systems, Differential Equations & Applications, June 25–28, Université de Poitiers, France, June 27.
52. J.A. GRIEPENTROG, *Nonlocal phase separation and image processing*, Workshop “PDE Approaches to Image Processing”, October 7–10, Universität Köln, October 9.
53. ———, *Global regularity for nonsmooth parabolic problems in Sobolev–Morrey spaces*, Mathematisches Kolloquium, Universität Rostock, November 30.
54. R. HENRION, *Quelques propriétés structurelles de contraintes en probabilité*, Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée, France, May 16.
55. ———, *Initiation aux contraintes en probabilité*, Electricité de France R&D, Clamart, France, May 17.

56. ———, *On chance constraints with random coefficient matrix*, 19th International Symposium on Mathematical Programming (ISMP 2006), Rio de Janeiro, Brazil, August 3.
57. ———, *Structural analysis for some basic types of probabilistic constraints*, Prague Stochastics 2006, Czech Republic, August 25.
58. ———, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen im operativen und strategischen Management von Wassernetzwerken*, Leibniz-Universität Hannover, September 7.
59. E. HOLZBECHER, *Hydraulic modelling with COMSOL/FEMLAB (block lecture)*, 15 talks, Polish Geological Institute, Pomeranian Branch, Szczecin, July 24–28.
60. ———, *Hydraulic modelling with COMSOL/FEMLAB (block lecture)*, 15 talks, Polish Geological Institute, Pomeranian Branch, Szczecin, October 9–13.
61. D. HÖMBERG, *Die Wärmebehandlung von Stahl — ein Optimierungsproblem*, Universität Bremen, SFB 570 “Distortion Engineering”, March 2.
62. ———, *Optimal control of thermomechanical phase transitions*, Workshop “Inverse and Control Problems for PDE’s”, March 13–17, Rome, Italy, March 13.
63. ———, *Modellierung, Simulation und Optimierung der Wärmebehandlung von Stahl*, Endress+Hauser Flowtec AG, Reinach, Switzerland, May 15.
64. ———, *Optimal control of laser material treatments*, 21st European Conference on Operational Research (EURO XXI), July 3–5, Reykjavik, Iceland, July 3.
65. ———, *Phasenübergänge in Stahl*, 5 talks, Summer School “Simulation und Anwendungen von Mikrostrukturen”, Föhr, August 14–18.
66. ———, *Optimal control of a thermomechanical phase transition model*, 12th IEEE International Conference on Methods and Models in Automation and Robotics, August 28–31, Miedzyzdroje, Poland, August 29.
67. ———, *Laser surface hardening — modelling, simulation and optimal control*, 4th Korean-German Seminar on Applied Mathematics and Physics, September 24 – October 1, Erlangen, September 26.
68. ———, *Thermomechanical models of phase transitions — modelling, control and industrial applications*, Escuela Politécnica Nacional, Departamento de Matemática, Quito, Ecuador, November 13.
69. ———, *A crash course in Nonlinear Optimization*, 12 talks, Escuela Politécnica Nacional, Quito, Ecuador, November 13–23.
70. O. KLEIN, *Outwards pointing properties for Preisach operators*, International Workshop on Multi-Rate Processes & Hysteresis (MURPHYS 2006), April 3–7, University College Cork, Ireland, April 4.
71. ———, *Asymptotic behavior for a phase-field model for thermo-visco-plasticity involving outwards pointing hysteresis operators*, 6th AIMS International Conference on Dynamical Systems, Differential Equations & Applications, June 25–28, Université de Poitiers, France, June 26.
72. A. KOŁODKO, *Iterative procedure for pricing callable options*, 4th Actuarial and Financial Mathematics Day, Brussels, Belgium, February 10.
73. TH. KOPRUCKI, *Modellierung und numerische Berechnung elektronischer Zustände in Halbleiter-Nanostrukturen*, Technische Universität Hamburg-Harburg, Institut für Numerische Simulation, May 17.
74. CH. KRAUS, *The sharp interface limit of the van der Waals–Cahn–Hilliard model*, Polish-German Workshop “Modeling Structure Formation”, Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Poland, September 8.
75. P. KREJČÍ, *A maximum principle in coupled evolution systems with applications to phase transition modeling*, Séminaire d’Équations aux Dérivées Partielles et Applications, Université de Poitiers, Mathématiques, France, February 16.

76. ———, *Hysteresis in temperature driven phase transition*, GAMM Annual Meeting 2006, March 29–31, Technische Universität Berlin, March 30.
77. ———, *Time scale doubling and asymptotic hysteresis in a phase separation problem*, International Workshop on Multi-Rate Processes & Hysteresis (MURPHYS 2006), April 3–7, University College Cork, Ireland, April 5.
78. ———, *Mathematics of remembering and forgetting (in Czech)*, Seminar on the History of Mathematics, Czech Technical University in Prague, Faculty of Civil Engineering, May 2.
79. ———, *Hysteresis wave propagation*, Seminario di Analisi, Università di Milano, Dipartimento di Matematica, Italy, June 13.
80. ———, *Long time dynamics of non-smooth phase-field systems*, Equazioni alle Derivate Parziali Modelli e Applicazioni, Università di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, June 15.
81. ———, *A thermodynamically consistent temperature-dependent Preisach hysteresis model*, 6th AIMS International Conference on Dynamical Systems, Differential Equations & Applications, June 25–28, Université de Poitiers, France, June 26.
82. CH. LECHNER, *Numerical simulation of Czocharlski crystal growth*, Seminar for Numerical Mathematics, Charles University in Prague, Faculty of Mathematics and Physics, Czech Republic, November 20.
83. P. MATHÉ, *Glattheit jenseits von Differenzierbarkeit*, Interdisciplinary Colloquium on Stochastics, Technische Universität Darmstadt, Fachbereich Mathematik, June 7.
84. ———, *Zur numerischen Analysis des Metropolis-Verfahrens*, Universität Bonn, September 22.
85. ———, *Glattheit jenseits Differenzierbarkeit*, Chemnitzer Mathematisches Kolloquium, Technische Universität Chemnitz, Fakultät für Mathematik, November 9.
86. ———, *Projektionsverfahren im Hilbertraum*, Research Seminar “Partielle Differentialgleichungen und Inverse Probleme”, Technische Universität Chemnitz, Fakultät für Mathematik, November 10.
87. ———, *Discretization of inverse problems*, Mini-Workshop on Statistical Methods for Inverse Problems, November 26 – December 2, Mathematisches Forschungsinstitut Oberwolfach, November 28.
88. CH. MEYER, *Optimal control of PDEs with pointwise state constraints*, University of Warsaw, Interdisciplinary Centre for Mathematical and Computational Modelling, Poland, September 8.
89. ———, *Finite element error analysis for state-constrained optimal control problems*, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, November 14.
90. ———, *Finite element approximation of optimal control problems with pointwise state constraints*, Karl-Franzens-Universität, Institut für Mathematik und Wissenschaftliches Rechnen, Graz, Austria, November 21.
91. A. MIELKE, *Evolution of microstructures in shape-memory alloys*, Workshop “Modelling and Analysis of Phase Transitions”, January 19–21, Centro di Ricerca Matematica Ennio De Giorgi, Pisa, Italy, January 21.
92. ———, *The multiscale analysis of wave propagation in discrete, periodic lattices*, Symposium of the DFG Collaborative Research Center SFB 555 “Complex Non-linear Processes”, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, May 5.
93. ———, *Passage from atomic to continuous systems*, Senior Seminar ANALYSIS, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, May 23.
94. ———, *Gamma convergence for evolutionary problems*, Workshop “Applications of Asymptotic Analysis”, June 18–24, Mathematisches Forschungsinstitut Oberwolfach, June 20.
95. ———, *Multiscale methods for pulse propagation in discrete lattices*, 6th AIMS International Conference on Dynamical Systems, Differential Equations & Applications, June 25–28, Université de Poitiers, France, June 28.

96. ———, *Multiple scales and Gamma limits in rate-independent material models*, Berlin-Leipzig Seminar on Analysis and Probability Theory, Universität Leipzig, July 7.
97. ———, *Evolution of microstructures in shape-memory alloys*, Polish-German Workshop “Modelling Structure Formation”, Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Poland, September 8.
98. ———, *Two-scale modelling for Hamiltonian systems: Formal and rigorous results*, Workshop “PDE and Materials”, September 25–29, Mathematisches Forschungsinstitut Oberwolfach, September 26.
99. ———, *Deriving modulation equations via Lagrangian and Hamiltonian reduction*, Workshop “Mathematical Theory of Water Waves”, November 13–17, Mathematisches Forschungsinstitut Oberwolfach, November 14.
100. M. KRUŽÍK, A. MIELKE, T. ROUBÍČEK, *Modeling of hysteresis in shape-memory alloys via microstructure evolution*, European Conference on Smart Systems (Final Meeting of the Research Training Network “New Materials, Adaptive Systems and their Nonlinearities: Modelling, Control and Numerical Simulation”), October 26–28, Rome, Italy, October 27.
101. H.-J. MUCHA, *On validation of hierarchical clustering*, 30th Annual Meeting of Gesellschaft für Klassifikation (GfKl), March 8–10, Freie Universität Berlin, March 10.
102. ———, *About pairwise data clustering*, 25th Biennial Meeting of the Society for Multivariate Analysis in the Behavioural Sciences (SMABS) and 2nd Conference of the European Association of Methodology (EAM), July 2–5, Budapest, Hungary, July 3.
103. H. NEIDHARDT, *Perturbation theory of semigroups and evolution equations*, Jahrestagung der Deutschen Mathematiker-Vereinigung 2006, September 18–21, Universität Bonn, September 20.
104. ———, *Classical solutions of van Roosbroeck’s semiconductor equations*, Conference “Mathematical aspects of quantum transport in mesoscopic systems”, December 18–20, Université de Toulon et Centre de Physique Théorique, Marseille, France, December 18.
105. J. POLZEHL, *Structural adaptive smoothing by propagation-separation*, 69th Annual Meeting of the IMS and 5th International Symposium on Probability and its Applications, July 30 – August 4, Rio de Janeiro, Brazil, July 30.
106. J. RADEMACHER, *Towards macro-limits of Riemann problems in atomic chains*, GAMM Annual Meeting 2006, March 27–31, Technische Universität Berlin, March 30.
107. ———, *Modulated wave trains in Riemann problems of atomic chains*, Workshop on Dynamics of Nonlinear Waves, April 24–28, University of Groningen, Department of Mathematics and Computer Science, The Netherlands, April 27.
108. ———, *Macroscopic limits of atomic chains and modulated wave trains*, Workshop on Limit Problems in Analysis, May 1–5, Free University of Amsterdam, Faculty of Sciences, Leiden, The Netherlands, May 4.
109. ———, *Computing absolute and essential spectra using continuation*, Senior Seminar “Numerik”, Universität Bielefeld, Fakultät für Mathematik, May 17.
110. ———, *The saddle-node of nearly homogeneous wave trains in reaction-diffusion systems*, SIAM Conference on Analysis of Partial Differential Equations, July 9–12, Boston, MA, USA, July 11.
111. M. RADZIUNAS, *Agreement between cavity modes in traveling wave and Lang–Kobayashi models of laser with delayed feedback*, Cross-disciplinary Physics Seminar, Mediterranean Institute for Advanced Studies (IMEDEA), Palma de Mallorca, Spain, May 9.
112. ———, *Reduction and numerical bifurcation analysis of a PDE model for multisection lasers*, 6th Crimean School and Workshops “Nonlinear Dynamics, Chaos and Applications”, May 15–26, Yalta, Crimea, Ukraine, May 22.
113. A. RATHSFELD, *Sensitivity analysis for scatterometry and reconstruction of periodic grating structures*, Physikalisch-Technische Bundesanstalt, Berlin, October 26.

114. ———, *Inverses Problem, Sensitivitätsanalyse, optimierte Messstrategie*, BMBF-Projekttreffen ABBILD, Physikalisch-Technische Bundesanstalt, Berlin, November 13.
115. ———, *Sensitivity analysis for scatterometry and reconstruction of periodic grating structures*, University of Delaware, Department of Mathematical Sciences, Newark, USA, November 27.
116. J. REHBERG, *The Schrödinger–Poisson system*, Colloquium in Honor of Prof. Demuth, September 10–11, Universität Clausthal, September 10.
117. ———, *Regularity for nonsmooth elliptic problems*, Crimean Autumn Mathematical School, September 20–25, Vernadskiy Tavricheskiy National University, Laspi, Ukraine, September 21.
118. K.K. SABELFELD, *Stochastic methods for solving PDEs with random parameters*, Kolloquium über Angewandte und Numerische Mathematik, Eidgenössische Technische Hochschule Zürich, Institut für Mathematik, Switzerland, May 3.
119. ———, *Randomized and Fourier/wavelet models for multi-dimensional Gaussian random fields*, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, June 15.
120. ———, *Random field simulation and applications*, 7th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (MCQMC 2006), August 14–18, Universität Ulm, August 17.
121. G. SCHMIDT, *Regularity of solutions to anisotropic elliptic transmission problems*, University of Liverpool, Department of Mathematical Sciences, UK, October 25.
122. J.G. SCHOENMAKERS, *Iterative procedures for the Bermudan stopping problem*, 42nd Dutch Mathematical Congress, March 27–28, Delft University of Technology, Faculty of Electrical Engineering, Mathematics and Computer Science, The Netherlands, March 27.
123. ———, *Interest rate modelling: Practical calibration and implementation techniques*, 2 talks, Risk, London, UK, June 15–16.
124. H. SI, *Mesh generation techniques*, Technische Universität Carolo-Wilhelmina zu Braunschweig, Institut für Wissenschaftliches Rechnen, March 3.
125. ———, *Constrained Delaunay tetrahedralization: Construction and refinement*, Carnegie Mellon University, Department of Mathematical Sciences, Pittsburgh, USA, September 26.
126. V. SPOKOINY, *Local parametric modeling*, Hejnice Compact Seminar (Collaborative Research Center SFB 649 “Economic Risk”), February 10–12, International Centre for Spiritual Rehabilitation, Hejnice, Czech Republic, February 12.
127. ———, *Adaptive local parametric approach to nonparametric estimation*, University of Bristol, Department of Mathematics, UK, February 24.
128. ———, *Adaptive estimation by local change point analysis with applications to analysis of nonstationary financial time series*, London School of Economics, Department of Statistics, UK, March 3.
129. ———, *Adaptive local likelihood modeling with applications to imaging*, Technion —Israel Institute of Technology, Department of Computer Science, Haifa, March 20.
130. ———, *In search of non-Gaussian components of a high-dimensional distribution*, Technion —Israel Institute of Technology, Department of Computer Science, Haifa, March 23.
131. ———, *Local parametric methods in nonparametric estimation*, 3 talks, Universität Heidelberg, May 4.
132. ———, *Local parametric approach to nonparametric estimation*, Special Statistics Colloquium, University of Maryland, Department of Mathematics, USA, November 16.
133. ———, *Adaptive estimation in statistical inverse problems*, Mini-Workshop on Statistical Methods for Inverse Problems, November 26 – December 2, Mathematisches Forschungsinstitut Oberwolfach, November 28.

134. ———, *Adaptive local parametric approach to nonparametric estimation*, Workshop on Image Analysis and Inverse Problems, December 11–12, EURANDOM, Eindhoven, The Netherlands, December 11.
135. J. SPREKELS, *The control variational method*, Università degli Studi di Firenze, Dipartimento di Matematica “U. Dini”, Italy, April 21.
136. ———, *Phase field models for phase transitions and applications*, 6 talks, Università di Roma “La Sapienza”, Dipartimento di Matematica, Italy, April 26–28.
137. ———, *The control variational method*, Università degli Studi di Milano, Dipartimento di Matematica “F. Enriques”, Italy, May 9.
138. ———, *The control variational method*, Università di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, May 16.
139. ———, *Asymptotics of the stop hysteresis operator*, Workshop “Applications of Asymptotic Analysis”, June 18–22, Mathematisches Forschungsinstitut Oberwolfach, June 21.
140. ———, *Prandtl–Ishlinskii hysteresis operators and 1D elastoplasticity*, 6th AIMS International Conference on Dynamical Systems, Differential Equations & Applications, June 25–28, Université de Poitiers, France, June 26.
141. ———, *The von Mises model for one-dimensional elastoplastic beams and Prandtl–Ishlinskii hysteresis operators*, Recent Advances in Free Boundary Problems and Related Topics (FBP 2006), September 14–16, Levico Terme, Italy, September 16.
142. ———, *On the asymptotic behaviour of the stop hysteresis operator*, Evolution Equations: Direct and Inverse Problems, September 18–20, Università di Bologna, Dipartimento di Matematica, Italy, September 20.
143. K. TABELOW, *Analyzing fMRI experiments with structural adaptive smoothing methods*, BCCN PhD Symposium 2006, June 7–8, Bernstein Center for Computational Neuroscience Berlin, Bad Liebenwalde, June 8.
144. A. VLADIMIROV, *Dynamics of light pulses in mode-locked lasers*, 6th Crimean School and Workshops “Non-linear Dynamics, Chaos and Applications”, May 15–26, Yalta, Crimea, Ukraine, May 20.
145. ———, *Nonlinear dynamics and bifurcations in multimode and spatially distributed laser systems*, June 20–23, St. Petersburg State University, Russia, June 20.
146. ———, *Transverse Bragg dissipative solitons in a Kerr cavity with refractive index modulation*, Laser Optics Conference, June 26–30, St. Petersburg, Russia, June 28.
147. ———, *Nonlinear dynamics in multimode and spatially extended laser systems*, Moscow State University, Physics Faculty, Russia, November 10.
148. V. WACHTEL, *On the sum of independent variables without power moments*, Russian Academy of Sciences, Sobolev Institute of Mathematics, Novosibirsk, April 20.
149. ———, *Lower deviation probabilities for supercritical Galton–Watson processes*, 9th International Vilnius Conference on Probability Theory and Mathematical Statistics, June 25–30, Vilnius Gediminas Technical University (VGTU), Lithuania, June 26.
150. ———, *Lower deviation probabilities for supercritical Galton–Watson processes*, IV Conference on Limit Theorems in Probability Theory and Their Applications, August 21–25, Novosibirsk State University, Institute of Mathematics, Department of Probability and Statistics, Russia, August 21.
151. B. WAGNER, *Slippage and viscoelastic effects for dewetting films*, Workshop on Thin Films and Fluid Interfaces, January 30 – February 2, Institute for Pure and Applied Mathematics, University of California, Los Angeles, USA, February 1.
152. ———, *Modellierung und asymptotische Analyse des Entnetzungsprozesses dünner Schichten*, Mathematische Modellierung in den Naturwissenschaften, Universität Hamburg, Fachbereich Mathematik, December 19.

153. A. MÜNCH, B. WAGNER, *Slippage effects for dewetting films*, Autumn Workshop 2006 of the Priority Program SPP 1164 “Nano- and Microfluidics: Bridging the Gap between Molecular Motion and Continuum Flow”, October 4–6, Bad Honnef, October 5.
154. W. WAGNER, *Explosion phenomena in stochastic coagulation-fragmentation models*, University of Cambridge, Centre for Mathematical Sciences, UK, May 9.
155. ———, *Acceptance-rejection techniques for the Maxwellian inflow distribution*, 7th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (MCQMC 2006), August 14–18, Universität Ulm, August 14.
156. ———, *Stochastic models and numerical algorithms for the Boltzmann equation*, Boltzmann Symposium, October 11–13, Ludwig-Maximilians-Universität München, Mathematisches Institut, October 12.
157. A. WEISS, *Escaping the Brownian stalkers*, BRG Workshop on Stochastic Models from Biology and Physics, October 9–10, Johann Wolfgang Goethe-Universität Frankfurt, October 10.
158. M. WOLFRUM, *Dynamics of chemical systems with mass action kinetics*, Colloquium in Memory of Karin Gatermann, Universität Hamburg, Fachbereich Mathematik, January 7.
159. ———, *Systems of delay differential equations with large delay*, Seminário do Centro de Análise Matemática, Geometria e Sistemas Dinâmicos, Instituto Superior Técnico, Departamento de Matemática, Lisbon, Portugal, March 28.
160. ———, *Instabilities of laser systems with delay*, 6th Crimean School and Workshops “Nonlinear Dynamics, Chaos and Applications”, May 15–26, Yalta, Crimea, Ukraine, May 19.
161. ———, *Describing a class of global attractors via symbol sequences*, 6th AIMS International Conference on Dynamical Systems, Differential Equations & Applications, June 25–28, Université de Poitiers, France, June 28.
162. S. YANCHUK, *Bifurcations in systems with long delay*, Seminar of the Magnetoencephalography (MEG) Group, Research Center Jülich, Institute of Medicine, April 19.
163. ———, *Typical instabilities in systems with large delay*, 6th Crimean School and Workshops “Nonlinear Dynamics, Chaos and Applications”, May 15–26, Yalta, Crimea, Ukraine, May 24.

A.8.2 Talks for a More General Public

1. U. BANDELOW, *Analysis of effects in optoelectronics and photonics*, Trade Fair and Congress Laser-Optik-Berlin (LOB) 2006, March 23–24, Studio Berlin GmbH, March 23.
2. B. GENTZ, *Die Mathematik der Eiszeiten*, 11. Berliner Tag der Mathematik (11th Berlin Day of Mathematics), Technische Universität Berlin, May 6.
3. J.A. GRIEPENTROG, *Kontrastverstärkung in Bildern und optimale Flächenteilung*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2006, WIAS, Berlin, May 13.
4. A. MIELKE, *Mathematische Vermehrung von Mengen, Flächen, Volumen und Geld?*, 11. Berliner Tag der Mathematik (11th Berlin Day of Mathematics), Technische Universität Berlin, May 6.
5. J. RADEMACHER, *Orientierung für das Listing-Möbiusband*, 11. Berliner Tag der Mathematik (11th Berlin Day of Mathematics), Technische Universität Berlin, May 6.
6. J. SPREKELS, *Handys, Lote und Kristalle*, Fest der Mathematik (Festival of Mathematics) on the occasion of the opening of the Berlin Mathematical School and the renewed funding of the DFG Research Center MATHEON for four more years, Technische Universität Berlin, November 16.
7. K. TABELOW, *Den Gedanken auf der Spur*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2006, WIAS, Berlin, May 13.

8. W. WEISS, *Geschichten der Thermodynamik und obskure Anwendungen des zweiten Hauptsatzes*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2006, WIAS, Berlin, May 13.
9. ———, *Interessantes und Obskures zum ersten und zweiten Hauptsatz der Thermodynamik*, MathInside – alles Mathematik, event of the DFG Research Center MATHEON, Urania, Berlin, November 21.

A.8.3 Posters

1. K. AFANASIEV, P.L. EVANS, A. MÜNCH, B. WAGNER, *Modelling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces*, Evaluation Colloquium of the DFG Research Center MATHEON, Berlin, January 24–25.
2. U. BANDELOW, A. DEMIRCAN, A. MIELKE, M. PIETRZYK, *Nonlocal and nonlinear effects in fiber optics*, Evaluation Colloquium of the DFG Research Center MATHEON, Berlin, January 24–25.
3. M. BARO, H.-CHR. KAISER, J. REHBERG, *Quantum mechanical & macroscopic models for optoelectronic devices*, Evaluation Colloquium of the DFG Research Center MATHEON, Berlin, January 24–25.
4. A. DEMIRCAN, U. BANDELOW, *Compression limit by third-order dispersion in the normal dispersion regime*, 14th European Conference on Mathematics for Industry (ECMI 2006), Universidad Carlos III de Madrid, Spain, July 10–14.
5. W. DREYER, F. DUDERSTADT, M. HERRMANN, S.-J. KIMMERLE, M. NALDZHIEVA, B. NIETHAMMER, *Macroscopic models for precipitation in crystalline solids*, Evaluation Colloquium of the DFG Research Center MATHEON, Berlin, January 24–25.
6. J. FUHRMANN, G. ENCHERY, A. BRADJI, U. BAYER, F. MARGI, *Verification of thermohaline simulations*, 5th Colloquium of the DFG Priority Program SPP 1135 “Dynamics of Sedimentary Systems under Varying Stress Regimes: The Example of the Central European Basin”, Geseke-Eringerfeld, November 15–17.
7. K. GÄRTNER, A. GLITZKY, TH. KOPRUCKI, *Analysis and simulation of spin-polarized drift-diffusion models*, Evaluation Colloquium of the DFG Priority Program SPP 1285 “Semiconductor Spintronics”, Bad Honnef, December 14–15.
8. A. GLITZKY, R. NÜRNBERG, U. BANDELOW, *WIAS-TeSCA: Simulation of semiconductor lasers*, Laser-Optik-Berlin, March 23–24.
9. J.A. GRIEPENTROG, *Anwendung eines nichtlokalen Phasenseparationsmodells zur Bildverwertung in der Rheumadiagnostik*, BMBF Status Seminar “Mathematik für Innovationen in Industrie und Dienstleistungen”, December 13–14.
10. A. EICHORN, R. HENRION, W. RÖMISCH, *Mean-risk optimization of electricity production in liberalized markets*, Evaluation Colloquium of the DFG Research Center MATHEON, Berlin, January 24–25.
11. E. HOLZBECHER, J. FUHRMANN, *Modelling of a differential electrochemical mass spectroscopy flow cell*, Workshop “Scientific Advances in Fuel Cell Systems”, Turin, Italy, September 13–14.
12. D. HÖMBERG, D. KERN, F. TRÖLTZSCH, *Modelling and optimization of phase transitions in steel*, Evaluation Colloquium of the DFG Research Center MATHEON, Berlin, January 24–25.
13. ———, *Modelling and optimization of phase transitions in steel*, Indo-German Workshop on Automatic Differentiation, Optimal Control and Adaptivity with Applications (ADOCOA-06), Indian Institute of Technology Bombay, India, November 11–17.
14. R. KRAUSE, D. HÖMBERG, J. SPREKELS, *Optimal control of a coupled thermo-electromagnetic evolution problem using non-conforming domain decomposition techniques*, Evaluation Colloquium of the DFG Priority Program SPP 1253 “Optimization with Partial Differential Equations”, Bad Honnef, February 6–8.
15. O. KLEIN, CH. LECHNER, P.-E. DRUET, *Numerical simulation of VCz growth with a traveling magnetic field*, 5th International Workshop on Modeling in Crystal Growth, Bamberg, September 10–13.

16. J. GEISER, O. KLEIN, P. PHILIP, *Numerical simulation of temperature fields during the sublimation growth of SiC single crystals using WIAS-Hi TNIHS*, 5th International Workshop on Modeling in Crystal Growth, Bamberg, September 10–13.
17. D. KNEES, A. MIELKE, *Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys*, Evaluation Colloquium of the DFG Research Center MATHEON, Berlin, January 24–25.
18. P. PHILIP, *A quasistatic crack propagation model allowing for cohesive forces and crack reversibility*, Recent Advances in Free Boundary Problems and Related Topics (FBP2006), Levico, Italy, September 14–16.
19. M. RADZIUNAS, T. KÖHLER, *LDSE-tool: Simulation and analysis of dynamics in semiconductor lasers*, Laser-Optik-Berlin, March 23–24.
20. M. LICHTNER, M. RADZIUNAS, L. RECKE, M. WOLFRUM, *Nonlinear dynamical effects in integrated optoelectronic structures*, Evaluation Colloquium of the DFG Research Center MATHEON, Berlin, January 24–25.
21. J. REHBERG, *Existence and uniqueness for van Roosbroeck's system in Lebesgue spaces*, Conference “Recent Advances in Nonlinear Partial Differential Equations and Applications”, Toledo, Spain, June 7–10.
22. A. SEGATTI, *On the hyperbolic relaxation of the Cahn–Hilliard equation in 3D*, Recent Advances in Free Boundary Problems and Related Topics (FBP2006), Levico, Italy, September 14–16.
23. K. TABELOW, *Image and signal processing in medicine and biosciences*, Evaluation Colloquium of the DFG Research Center MATHEON, Berlin, January 24–25.
24. ———, *Structure adaptive smoothing in statistical fMRI analysis*, Workshop “Highfield MRI and MRS-3T and Beyond”, Physikalisch-Technische Bundesanstalt Berlin, February 20–21.
25. K. TABELOW, J. POLZEHL, H.U. VOSS, V. SPOKOINY, *Analyzing fMRI experiments with structural adaptive smoothing methods*, Human Brain Mapping Conference, Florence, Italy, June 12–15.
26. K. TABELOW, J. POLZEHL, V. SPOKOINY, J.P. DYKE, L.A. HEIER, H.U. VOSS, *Accurate localization of functional brain activity using structure adaptive smoothing*, ISMRM 14th Scientific Meeting & Exhibition, Seattle, USA, May 10–14.
27. A. WEISS, *Microscopic modelling of complex financial assets*, Evaluation Colloquium of the DFG Research Center MATHEON, Berlin, January 24–25.
28. W. WEISS, *WIAS-SHarp: Surface hardening program*, Laser-Optik-Berlin, March 23–24.

A.9 Visits to other Institutions⁴

1. CH. BENDER, Technische Universität Braunschweig, Institut für Mathematische Stochastik, November 1, 2005 – February 28, 2006.
2. ———, Helsinki University of Technology, Institute of Mathematics, Finland, March 1–10.
3. M. BIRKNER, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, January 23–26.
4. ———, CNRS–Centre de Physique Théorique, Marseille, France, February 15–18.
5. ———, Universität Bielefeld, Technische Fakultät, September 4–20.
6. A. BOVIER, Technion – Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, December 17, 2005 – January 8, 2006.
7. ———, École Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, March 20 – April 14.
8. ———, Università degli Studi di Firenze, Dipartimento di Fisica, Italy, June 7–11.
9. ———, University of Leiden, Mathematics & Natural Sciences, The Netherlands, September 21 – October 1.
10. ———, Technion – Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, December 19, 2006 – January 2, 2007.
11. N. CHAMPAGNAT, Université Paris VI, Laboratoire de Probabilités et Modèles Aléatoires, France, February 28 – March 5.
12. A. DEMIRCAN, University of Bath, Department of Physics, Centre for Photonics and Photonic Materials, UK, August 14–25.
13. W. DREYER, Università degli Studi di Trento, Dipartimento di Matematica, Italy, February 6–10.
14. P.-É. DRUET, Nečas Center for Mathematical Modeling, Prague, Czech Republic, November 2 – December 1.
15. J. ELSCHNER, University of Tokyo, Department of Mathematical Sciences, Japan, February 7–24.
16. ———, Universität Karlsruhe, Institut für Mathematik, October 16–20.
17. M. FISCHER, Università di Roma “La Sapienza”, Dipartimento di Economia, Italy, April 1 – September 30.
18. K. FLEISCHMANN, University of Bath, Department of Mathematical Sciences, and University of Oxford, Mathematical Institute, UK, March 3–11.
19. ———, Technion – Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, April 23 – May 3.
20. P. GAPEEV, Helsinki University of Technology, Institute of Mathematics, Finland, October 2–13.
21. ———, Université Paris VI, Laboratoire de Probabilités et Modèles Aléatoires, France, November 8–22.
22. B. GENTZ, CNRS–Centre de Physique Théorique, Marseille, France, June 4–16.
23. R. HENRION, Électricité de France R&D, Clamart, France, May 15–22.
24. ———, Université d’Avignon, Département de Mathématiques, France, November 24 – December 5.
25. D. HÖMBERG, Escuela Politécnica Nacional, Departamento de Matemática, Quito, Ecuador, November 13–23.
26. D. KERN, Universität Münster, Institut für Numerische und Angewandte Mathematik, September 11–15.
27. P. KREJČÍ, Institut National de Recherche en Informatique et en Automatique (INRIA), Rocquencourt, France, February 7 – March 4.

⁴Only stays of more than three days are listed.

28. CH. LECHNER, Nečas Center for Mathematical Modeling, Prague, Czech Republic, November 5 – December 6.
29. P. MATHÉ, Friedrich-Schiller-Universität Jena, Fakultät für Mathematik und Informatik, July 24–27.
30. ———, Technische Universität Chemnitz, Fakultät für Mathematik, November 6–10.
31. CH. MEYER, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, November 13–17.
32. ———, Karl-Franzens-Universität Graz, Institut für Mathematik, Austria, November 20–23.
33. C. PATZ, CERMICS-ENPC: Centre d’Enseignement et de Recherche en Mathématiques et Calcul Scientifique – Ecole Nationale des Ponts et Chaussées, Paris, France, June 23–30.
34. J. POLZEHL, University of Minnesota, School of Statistics, Minneapolis, USA, June 12–30.
35. M. RADZIUNAS, Universitat de les Illes Balears, Departament de Física, Palma de Mallorca, Spain, May 8–17.
36. A. RATHSFELD, University of Delaware, Department of Mathematical Sciences, Newark, USA, November 20–29.
37. K.K. SABELFELD, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, June 12 – July 21.
38. ———, Universität Ulm, Fakultät für Informatik, August 21–25.
39. ———, Institut National de Recherche en Informatique et en Automatique (INRIA), Sophia-Antipolis, France, September 6–14.
40. ———, Universität Siegen, Fachbereich Mathematik, October 11–17.
41. F. SCHMID, Instituto Superior Tecnico, Lisbon, Portugal, June 10–18.
42. G. SCHMIDT, University of Liverpool, Department of Mathematical Sciences, UK, October 23–27.
43. V. SPOKOINY, London School of Economics, Department of Statistics, UK, February 19 – March 3.
44. ———, University of Haifa, Department of Statistics, Israel, March 20 – April 3.
45. ———, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, August 28 – September 22.
46. ———, University of Maryland, Department of Mathematics, USA, November 15–18.
47. J. SPREKELS, Università degli Studi di Firenze, Dipartimento di Matematica “Ulisse Dini”; Università di Roma “La Sapienza”, Dipartimento di Matematica; Università di Pavia, Dipartimento di Matematica “F. Casorati”; Università degli Studi di Milano, Dipartimento di Matematica “F. Enriques”, Italy, April 20 – May 19.
48. A. VLADIMIROV, St. Petersburg State University, General Physics Department-1, Russia, June 20–23.
49. B. WAGNER, Technische Universität Berlin, Institut für Mathematik, April 1 – September 30.
50. W. WAGNER, Universität des Saarlandes, Fachbereich Mathematik, Saarbrücken, March 27–30.
51. ———, University of Cambridge, Statistical Laboratory and Department of Engineering, UK, May 8 – June 1.
52. ———, Università di Catania, Dipartimento di Matematica e Informatica, Italy, June 17–24.
53. M. WOLFRUM, Technical University of Lisbon, Department of Mathematics, Portugal, March 26 – April 4.
54. S. YANCHUK, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, May 8–12.

A.10 Academic Teaching⁵

Winter Semester 2005/2006

1. L. RECKE, H.-J. WÜNSCHE, U. BANDELOW, *Mathematische Modelle der Photonik* (seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.
2. CH. BENDER, *Finanzmathematik* (lecture), Technische Universität Braunschweig, 4 SWS.
3. ———, *Finanzmathematik* (exercises), Technische Universität Braunschweig, 2 SWS.
4. M. BIRKNER, *Mathematik I für Brauerei- und Brennereitechnologen* (lecture), Technische Universität Berlin, 2 SWS.
5. ———, *Mathematik I für Brauerei- und Brennereitechnologen* (exercises), Technische Universität Berlin, 1 SWS.
6. A. BOVIER, *Extrema stochastischer Folgen und Prozesse* (lecture), Technische Universität Berlin, 2 SWS.
7. A. BOVIER, B. GENTZ, H. FÖLLMER, P. IMKELLER, U. KÜCHLER, J.-D. DEUSCHEL, J. GÄRTNER, M. SCHEUTZOW, A. SCHIED, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Technische Universität Berlin, 2 SWS.
8. C. CARSTENSEN, J. GEISER, *Diskretisierungs- und Lösungsverfahren für parabolische Differentialgleichungen: Theorie und Anwendungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
9. B. GENTZ, *Große Abweichungen – Theorie und Anwendungen* (lecture), Technische Universität Berlin, 2 SWS.
10. A. GLITZKY, *Einführung in die Kontrolltheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
11. J.A. GRIEPENTROG, *Evolutionsgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
12. R. HENRION, W. RÖMISCH, M. STEINBACH, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
13. E. HOLZBECHER, *Grundwassermodellierung I* (lecture), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
14. ———, *Grundwassermodellierung I* (exercises), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
15. D. HÖMBERG, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
16. ———, *Spieltheorie* (seminar), Technische Universität Berlin, 2 SWS.
17. A. MIELKE, *Höhere Analysis I (Funktionalanalysis)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
18. H. GAJEWSKI, B. NIETHAMMER, A. MIELKE, J. SPREKELS, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
19. V. SPOKOINY, *Modern Nonparametric Modelling* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
20. V. SPOKOINY, W. HÄRDLE, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
21. J. SPREKELS, *Analysis IV* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
22. H. GAJEWSKI, J. SPREKELS, F. TRÖLTZSCH, R. KLEIN, CH. SCHÜTTE, P. DEUFLHARD, R. KORNUBER, OTHERS, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS.
23. H. STEPHAN, *Kombinatorik und Wahrscheinlichkeitstheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
24. K. TABELOW, *Mathematik und Elektrotechnik* (seminar), Deutsches Herzzentrum Berlin, Akademie für Kardiotechnik, 4 SWS.
25. M. WOLFRUM, J. HÄRTERICH, *Nichtlineare Dynamik* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

⁵SWS = semester periods per week

Summer Semester 2006

1. L. RECKE, H.-J. WÜNSCHE, U. BANDELOW, *Mathematische Modelle der Photonik* (seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.
2. CH. BENDER, *Zinsmodelle* (lecture), Justus-Liebig-Universität Gießen, 2 SWS.
3. A. BOVIER, *Wahrscheinlichkeitstheorie I* (lecture), Technische Universität Berlin, 4 SWS.
4. A. BOVIER, B. GENTZ, H. FÖLLMER, P. IMKELLER, U. KÜCHLER, J.-D. DEUSCHEL, J. GÄRTNER, M. SCHEUTZOW, A. SCHIED, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
5. W. DREYER, *Projekt Nichtlineare Kontinuumsmechanik* (lecture), Technische Universität Berlin, Institut für Mechanik, 4 SWS.
6. R. HENRION, W. RÖMISCH, M. STEINBACH, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
7. E. HOLZBECHER, *Grundwassermodellierung I* (lecture), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
8. ———, *Grundwassermodellierung I* (exercises), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
9. D. HÖMBERG, *Optimalsteuerung bei partiellen Differentialgleichungen* (lecture), Technische Universität Berlin, 4 SWS.
10. P. MATHÉ, E. BEHRENDTS, *Statistik mit "R"* (seminar), Freie Universität Berlin, 2 SWS.
11. A. MIELKE, *Höhere Analysis II (Lineare partielle Differentialgleichungen)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
12. H. GAJEWSKI, B. NIETHAMMER, A. MIELKE, J. SPREKELS, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
13. V. SPOKOINY, *Methoden der nichtparametrischen Statistik* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
14. V. SPOKOINY, W. HÄRDLE, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
15. H. GAJEWSKI, J. SPREKELS, F. TRÖLTZSCH, R. KLEIN, CH. SCHÜTTE, P. DEUFLHARD, R. KORNUBER, OTHERS, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS.
16. H. STEPHAN, *Kombinatorik und additive Zahlentheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
17. K. TABELOW, *Mathematik und Elektrotechnik* (seminar), Deutsches Herzzentrum Berlin, Akademie für Kardiotechnik, 4 SWS.
18. B. WAGNER, *Analysis I für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
19. ———, *Analysis I für Ingenieure* (exercises), Technische Universität Berlin, 2 SWS.
20. M. WOLFRUM, J. HÄRTERICH, *Nichtlineare Dynamik* (senior seminar), Freie Universität Berlin/WIAS, 2 SWS.

Winter Semester 2006/2007

1. U. BANDELOW, *Mechanik und Wärmelehre* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
2. L. RECKE, H.-J. WÜNSCHE, U. BANDELOW, *Mathematische Modelle der Photonik* (seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.
3. A. BOVIER, *Wahrscheinlichkeitstheorie II – BMS Basic Course Stochastic Processes I* (lecture), Technische Universität Berlin, 4 SWS.


4. A. BOVIER, H. FÖLLMER, P. IMKELLER, U. KÜCHLER, J.-D. DEUSCHEL, J. GÄRTNER, M. SCHEUTZOW, A. SCHIED, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Technische Universität Berlin, 2 SWS.
5. W. DREYER, *Projekt Nichtlineare Kontinuumsmechanik* (lecture), Technische Universität Berlin, Institut für Mechanik, 4 SWS.
6. A. GLITZKY, *Optimale Steuerung bei parabolischen Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
7. R. HENRION, W. RÖMISCH, M. STEINBACH, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
8. E. HOLZBECHER, *Grundwassermodellierung II* (lecture), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
9. ———, *Grundwassermodellierung II* (exercises), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
10. D. HÖMBERG, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
11. A. MIELKE, *Glattheit von Lösungen elliptischer Gleichungen und Variationsproblemen* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
12. H. GAJEWSKI, B. NIETHAMMER, A. MIELKE, J. SPREKELS, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
13. J.G. SCHOENMAKERS, *Einführung in die Stochastische Finanzmathematik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
14. V. SPOKOINY, *Nichtparametrische Methoden und ihre Anwendungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
15. V. SPOKOINY, W. HÄRDLE, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
16. H. STEPHAN, *Konvexe Analysis* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
17. K. TABELOW, *Mathematik und Elektrotechnik* (seminar), Deutsches Herzzentrum Berlin, Akademie für Kardiotechnik, 4 SWS.
18. M. WOLFRUM, J. HÄRTERICH, *Nichtlineare Dynamik* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

A.11 Weierstrass Postdoctoral Fellowship Program

In 2005, the Weierstrass Institute for Applied Analysis and Stochastics has launched the *Weierstrass Postdoctoral Fellowship Program* (see <http://www.wias-berlin.de/main/jobs/jobs/fellowship.html.en>). The institute offers postgraduate fellowships with a duration of six up to twelve months. These fellowships are designed to enable highly-qualified young scientists to participate in the research into the mathematical problems in the main fields of the institute and thus to further their education and training.

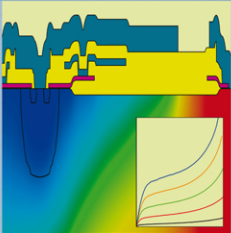
The fellowships can be started anytime in the year. The application deadlines are February 28 and August 31 of each year.

The fellowship holders in 2006 were Dr. Sergei Zelik (Institute for Information Transmission Problems, Russian Academy of Sciences), Dr. Robert Haller-Dintelmann (Technische Universität Darmstadt) and Dr. Xin Yao (Tsinghua University, Beijing, China).



Weierstrass Institute for Applied Analysis and Stochastics

Weierstrass Postdoctoral Fellowship Program



The Weierstrass Institute for Applied Analysis and Stochastics (WIAS) in Forschungsverbund Berlin e.V. (<http://www.wias-berlin.de>) is a research institute of the Leibniz Association. WIAS engages in project-oriented research in Applied Mathematics and ranks among the leading research institutions worldwide in the study of the mathematical aspects of the following fields:

- Nano- and optoelectronics
- Optimization and control of technological processes
- Phase transitions and multifunctional materials
- Stochastics in natural sciences and economic
- Flow and transport processes in continua
- Numerical methods of analysis and stochastics

WIAS offers postgraduate fellowships for 2007 and the following years. Their duration is six or twelve months. These fellowships are designed to enable highly-qualified young scientists to participate in the research into the mathematical problems in the above fields, thus furthering their education and training.

The fellowships can be started anytime in the year.

Application deadlines: February 28 and August 31 of each year. The decision on the applications will be taken within six weeks. The next application deadline is

August 31, 2007.

Value: The monthly stipend is 2,100 Euro. In well-founded cases, travel allowances may be paid, if a special application is made.

Qualifications for application: Applicants should hold a PhD in a subject relevant to one of the above fields. It is required that the candidates will have a good command of the German or English language.

Documents to be submitted with the application (in German or English):

- Curriculum vitae
- PhD certificate
- List of publications
- Summary of research activities to date and proposed research program
- Two letters of recommendation to be sent separately to the address given below

Applications should be sent to: Prof. Dr. Jürgen Sprekels, Director of WIAS, Mohrenstrasse 39, D-10117 Berlin, Germany (postdoc@wias-berlin.de).

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A.12 Visiting Scientists⁶

A.12.1 Guests

1. A. AMANN, Tyndall National Institute, Photonics Theory Group, Cork, Ireland, December 12–16.
2. K. AOKI, Kyoto University, Graduate School of Engineering, Department of Aeronautics and Astronautics, Japan, September 6 – October 5.
3. F. BAUER, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, August 10–19.
4. N. BERGLUND, CNRS Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique Théorique, Toulon, France, March 17 – April 15.
5. ———, July 24–28.
6. ———, August 28 – September 16.
7. A. BRADJI, Université de Provence, Centre de Mathématiques et Informatique (CMI), Marseille, France, February 14–17.
8. ———, March 15–31.
9. C. BUTUCEA, Université Paris VI “Pierre et Marie Curie”, Laboratoire de Probabilités et Modèles Aléatoires, France, April 11–22.
10. J. ČERNÝ, École Polytechnique Fédérale de Lausanne, Institut de Mathématiques, Switzerland, September 25 – October 20.
11. A.R. CHAMPNEYS, University of Bristol, Department of Engineering Mathematics, UK, May 23–26.
12. K. CHEŁMIŃSKI, Cardinal Stefan Wyszyński University, Faculty for Mathematics and Sciences, Warsaw, Poland, June 26 – July 21.
13. N. CHINO, Aichi Gakuin University, Department of Psychology, Japan, March 5–12.
14. R. CIEGIS, Vilnius Gedeminas Technical University, Department of Mathematical Modeling, Lithuania, October 29 – November 4.
15. P. CIZEK, Tilburg University, Department of Economics & OR, The Netherlands, October 15–20.
16. H. CORNEAN, Aalborg University, Department of Mathematical Sciences, Denmark, November 24 – December 9.
17. L. DE SANCTIS, International Center for Theoretical Physics, ICTP, Trieste, Italy, May 23–26.
18. D. DIVINE, Norwegian Polar Institute, Polar Environmental Centre, Tromsø, January 16 – July 15.
19. D. DUNCAN, Heriot-Watt University, School of Mathematical and Computer Sciences, Edinburgh, UK, May 1–21.
20. S.M. ERMAKOV, University of St. Petersburg, Faculty of Mathematics and Mechanics, Russia, October 30 – November 25.
21. P. EVANS, Humboldt-Universität zu Berlin, Institut für Mathematik, July 27, 2006 – December 31, 2009.
22. A. FAGGIONATO, Università di Roma “La Sapienza”, Dipartimento di Matematica, Italy, April 24 – May 5.
23. ———, September 3–11.
24. B. FERNANDEZ, CNRS Centre de Physique Théorique, CNRS Luminy, Marseille, France, July 24–28.
25. ———, August 28 – September 16.

⁶Only stays of more than three days are listed.

26. P. FERRARI, Technische Universität München, Zentrum Mathematik, Bereich M5, July 3–7.
27. ———, September 30 – October 7.
28. D. FLYNN, University College Cork, Department of Civil and Environmental Engineering, Ireland, May 6–21.
29. J. GIANNOULIS, Technische Universität München, Zentrum Mathematik, June 1 – September 30.
30. K. GLASNER, University of Arizona, Department of Mathematics, Santa Rita, USA, July 8–22.
31. Y. GOLUBEV, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, November 20 – December 8.
32. R.B. GUENTHER, Oregon State University, Mathematics Department, Corvallis, USA, October 7–27.
33. E. GUERRE, Université Paris VI “Pierre et Marie Curie”, Laboratoire de Statistique Théorique et Appliquée, France, June 26–30.
34. M. HAKER, Universität Lübeck, Institut für Neuro- und Bioinformatik, October 9–13.
35. D. HILHORST, Université Paris-Sud, Laboratoire d’Analyse Numérique, Orsay, France, April 23–27.
36. B. HOFMANN, Technische Universität Chemnitz, Fakultät für Mathematik, March 6–10.
37. O. HOVORKA, Drexel University, College of Engineering, Philadelphia, USA, October 5–12.
38. G.C. HSIAO, University of Delaware, Department of Mathematical Sciences, Newark, USA, July 2–29.
39. D. IOFFE, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, July 24 – August 22.
40. A. JUDITSKY, Université Joseph Fourier Grenoble I, Laboratoire de Modélisation et Calcul, France, January 3–13.
41. J. KAMPEN, Universität Heidelberg, Institut für Angewandte Mathematik, October 2 – December 31.
42. E. KHRUSLOV, B. Verkin Institute for Low Temperature Physics and Engineering (ILTPE), Kharkov, Ukraine, October 16 – November 15.
43. V. KIRK, University of Auckland, Department of Mathematics, New Zealand, May 19–27.
44. D. KLATTE, University of Zurich, Institute of Operations Research, Switzerland, January 2–5.
45. E. KNOBLOCH, University of California, Department of Physics, Berkeley, USA, May 22–26.
46. J. KOPFOVÁ, Silesian University in Opava, Mathematical Institute, Czech Republic, March 6–10.
47. ———, July 10–14.
48. R. KRÄMER, Technische Universität Chemnitz, Fakultät für Mathematik, June 26–30.
49. K. KRUMBIEGEL, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, July 31 – August 4.
50. K. KUHNEN, Universität des Saarlandes, Physik und Mechatronik, Saarbrücken, March 19 – April 14.
51. ———, November 19–25.
52. O. KURBANMURADOV, Turkmen State University, Physics and Mathematics Research Center, Ashkhabat, April 30 – June 3.
53. ———, October 21 – December 22.
54. I. KURKOVA, Université Paris VI “Pierre et Marie Curie”, Laboratoire de Probabilités et Modèles Aléatoires, France, February 8–15.
55. A. LAMBERT, Université Paris VI “Pierre et Marie Curie”, Laboratoire de Probabilités et Modèles Aléatoires, France, January 18–24.
56. F. LEGOLL, École Nationale des Ponts et Chaussées, Laboratoire d’Analyse des Matériaux et Identification, Marne-la-Vallée, France, December 6–11.

57. A. LEVYKIN, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, May 4–29.
58. ———, November 17 – December 16.
59. A. LINKE, DFG Research Center MATHEON, Berlin, January 1 – May 31.
60. M.M. MALAMUD, Donetsk National University, Department of Mathematics, Ukraine, December 8–13.
61. J.A. MARTINS, Instituto Superior Técnico, Departamento de Engenharia Civil, Lisboa, Portugal, October 5–21.
62. F. MÉHATS, Université de Rennes 1, Institut de Recherche Mathématique de Rennes (IRMAR), France, May 1–11.
63. R. MESSIKH, École Polytechnique Fédérale de Lausanne, Institut de Mathématiques, Switzerland, July 6–16.
64. G.N. MILSTEIN, Ural State University, Department of Mathematics, Ekaterinburg, Russia, March 1 – June 30.
65. P. MÖRTERS, University of Bath, Department of Mathematical Sciences, UK, July 23 – August 22.
66. C. MUELLER, University of Rochester, Department of Mathematics, USA, July 16–22.
67. O. MUSCATO, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, June 17–24.
68. L. MYTNIK, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, February 7–14.
69. P. NEFF, Technische Universität Darmstadt, Fachbereich Mathematik, November 5–10.
70. F. NIER, Université de Rennes 1, Institut de Recherche Mathématique de Rennes (IRMAR), France, October 16 – November 12.
71. M. NIZETTE, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, November 6–24.
72. F. ORTEGÓN GALLEGÓ, Universidad de Cádiz, Departamento de Matemáticas, Puerto Real, Spain, September 4–11.
73. J. OUTRATA, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, February 13 – March 4.
74. ———, December 6–21.
75. B. PATRA, Ecole Normale Supérieure de Cachan, France, June 2 – July 25.
76. C. PATZ, CERMICS, Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée, France, March 26–31.
77. S. PECERICENKO, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, April 17 – May 17.
78. O. PENROSE, Heriot-Watt University, School of Mathematical and Computer Sciences, Edinburgh, UK, May 21–25.
79. A. PETROV, Université Claude Bernard (Lyon I), Laboratoire MAPLY, France, June 15–20.
80. V. PETZET, Universität Bayreuth, Lehrstuhl für Ingenieurmathematik, February 12–24.
81. ———, October 16–20.
82. P. PHILIP, University of Minnesota, Institute for Mathematics and its Applications, Minneapolis, USA, July 7–21.
83. M. PIETRZYK, Berlin, October 21 – November 19.
84. D. POLISEVSKI, Romanian Academy, Institute of Mathematics “Simion Stoilov”, Bucharest, January 8–14.
85. A. POLITI, CRN Istituto dei Sistemi Complessi, Fiorentino, Italy, November 14–27.

86. J. RADEMACHER, Centre for Science and Information, Department Modelling, Analysis and Simulation, Amsterdam, The Netherlands, December 3–8.
87. B. RAJARATNAM, Cornell University, Statistical Science, Ithaca, USA, June 19 – July 7.
88. O. RASSKAZOV, University College Cork, Department of Applied Mathematics, Ireland, May 6–21.
89. M. REISS, Universität Heidelberg, Institut für Angewandte Mathematik, April 10–13.
90. W. RING, Karl-Franzens-Universität Graz, Institut für Mathematik, Austria, August 21 – September 17.
91. L. RINGSTADT-OLSEN, University of Tromsø, Department of Mathematics and Statistics, Norway, February 9 – May 19.
92. Y. RITOV, The Hebrew University of Jerusalem, Department of Statistics, Israel, October 11–19.
93. E. ROCCA, Università degli Studi di Milano, Dipartimento di Matematica “F. Enriques”, Italy, October 17 – November 10.
94. A. ROHDE, Universität Heidelberg, Institut für Angewandte Mathematik, September 15 – October 15.
95. N. ROSANOV, Institute for Laser Physics, St. Petersburg, Russia, January 19–22.
96. A. SAKAI, EURANDOM, Eindhoven, The Netherlands, January 23–27.
97. S. SAUTER, Universität Zürich, Institut für Mathematik, Switzerland, December 11–15.
98. H. SCHULZ-BALDES, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, May 24–28.
99. I. SHALIMOVA, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, February 24 – March 24.
100. ———, April 10 – May 10.
101. ———, November 13 – December 13.
102. A. SHISHKOV, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Donetsk, July 14–20.
103. J. SIEBER, University of Bristol, Department of Engineering Mathematics, UK, December 3–23.
104. D. SKRYABIN, University of Bath, Department of Physics, UK, July 9–14.
105. J. SOKOŁOWSKI, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, April 2–30.
106. CH. SPARBER, Universität Wien, Wolfgang Pauli Institut & Fakultät für Mathematik, Austria, August 29 – September 12.
107. S. SPERLICH, Universidad Carlos III de Madrid, Departamento de Estadística y Econometría, Spain, December 21, 2005 – January 20, 2006.
108. C. SPITONI, Università degli Studi di Roma “La Sapienza”, Dipartimento di Metodi e Modelli Matematici, Italy, May 15 – September 27.
109. R. SUN, EURANDOM, Eindhoven, The Netherlands, February 6–10.
110. I. SUSHKO, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, December 4–22.
111. R. SZALAI, University of Bristol, Department of Engineering Mathematics, UK, November 12–18.
112. D. TIBA, Romanian Academy, Institute of Mathematics, Bucharest, February 1–28.
113. ———, November 1–30.
114. M. TLIDI, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, November 19–26.
115. M. TRETYAKOV, University of Leicester, Department of Mathematics, UK, April 8 – May 7.
116. D. TURAEV, Ben Gurion University of the Negev, Department of Mathematics, Beer Sheva, Israel, July 7 – August 8.

117. S. VAN DE GEER, Eidgenössische Technische Hochschule Zürich, Institut für Mathematik, Switzerland, February 7–10.
118. I. VAN KEILEGOM, Université Catholique de Louvain, Institut de Statistique, Louvain-la-Neuve, Belgium, July 4–7.
119. V.A. VATUTIN, Steklov Mathematical Institute, Department of Discrete Mathematics, Moscow, Russia, November 1–30.
120. C. VIAL, Université Paris X, Laboratoire Modal'X, Nanterre, France, January 29 – February 3.
121. ———, May 28 – June 4.
122. P. VOGT, ifb AG, Köln, July 19–22.
123. A. WAKOLBINGER, Johann Wolfgang Goethe-Universität Frankfurt, Institut für Stochastik und Mathematische Informatik, August 27 – September 3.
124. G. WARNECKE, Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik, September 21–29.
125. M. WOLF, Universität Zürich, Institut für Empirische Wirtschaftsforschung, Switzerland, June 13–16.
126. J. XIONG, University of Tennessee, Department of Mathematics, Knoxville, USA, June 5 – July 2.
127. M. YAMAMOTO, University of Tokyo, Department of Mathematical Sciences, Japan, April 7–21.
128. ———, September 12 – October 5.
129. V.A. ZAGREBNOV, Université Aix-Marseille II, Centre de Physique Théorique, France, May 2–5.
130. H. ZHAO, DFG Research Center MATHEON, Berlin, January 1 – May 31.

A.12.2 Scholarship Holders

1. I. BOROVSKEYA, Russian Academy of Sciences, Institute for Mathematical Modelling, Moscow, DAAD Fellowship, October 1, 2005 – March 31, 2006.
2. M. ELEUTERI, Università degli Studi di Trento, Dipartimento di Matematica, Ph.D. Fellowship of the Istituto Nazionale di Alta Matematica, Rome, Italy, April 24 – June 30.
3. M. ELEUTERI, Università degli Studi di Trento, Dipartimento di Matematica, Italy, Postdoctoral Fellowship of the Department of Mathematics of Trento, July 1 – December 31.
4. R. HALLER-DINTELMANN, Technische Universität Darmstadt, FB 4 – Mathematik, Weierstrass Postdoctoral Fellowship Program, October 1, 2006 – September 30, 2007.
5. A. HRYN, Yanka Kupala State University of Grodno, Faculty of Mathematics, Belarus, DAAD Fellowship, October 1 – December 31.
6. C.-G. LEFTER, University of Iași, Department of Mathematics, Romania, Humboldt Research Fellowship, May 1, 2005 – April 30, 2006.
7. A. MÜNCH, Humboldt-Universität zu Berlin, Institut für Mathematik, Heisenberg Fellowship of the Deutsche Forschungsgemeinschaft (German Research Foundation), November 1, 2003 – October 31, 2008.
8. L. PANIZZI, Scuola Normale Superiore, Pisa, Italy, Postdoctoral Fellowship of the Scuola Normale Superiore, March 9, 2006 – April 9, 2007.
9. T. ROUBÍČEK, Charles University, Mathematical Institute, Prague, Czech Republic, Humboldt Research Fellowship, January 16 – February 17.
10. T. ROUBÍČEK, Charles University, Mathematical Institute, Prague, Czech Republic, Humboldt Research Fellowship, August 21 – September 21.

11. L. XU, Imperial College London, UK, DAAD Fellowship, June 1 – September 30.
12. X. YAO, Tsinghua University, Department of Automation, Beijing, PR China, Weierstrass Postdoctoral Fellowship Program, March 1, 2006 – March 31, 2007.
13. S. ZELIK, Institute for Information Transmission Problems, Russian Academy of Sciences, Moscow, Russia, Weierstrass Postdoctoral Fellowship Program, November 1, 2005 – July 31, 2006.

A.12.3 Doctoral Candidates and Post-docs supervised by WIAS Collaborators

1. M. AN DER HEIDEN, Technische Universität Berlin, doctoral candidate, since May 1, 2002.
2. A. DEPPERSCHMIDT, Technische Universität Berlin, doctoral candidate, since January 1, 2004.
3. A. KLIMOVSKI, Technische Universität Berlin, doctoral candidate, since June 1, 2003.
4. A. MAINIK, Universität Stuttgart, Institut für Analysis, Dynamik und Modellierung, Collaborative Research Center Sfb 404 “Multifield Problems”, doctoral candidate, February 1, 2005 – December 31, 2006.
5. C. PATZ, Universität Stuttgart, Institut für Analysis, Dynamik und Modellierung, doctoral candidate, January 1, 2005 – April 30, 2006.
6. F. SCHMID, Universität Stuttgart, Institut für Analysis, Dynamik und Modellierung, doctoral candidate, January 1, 2005 – February 28, 2006.

A.13 Guest Talks

1. A. AMANN, Tyndall National Institute, Photonics Theory Group, Cork, Ireland, *Inverse scattering approach to multiwavelength Fabry–Perot laser design*, December 14.
2. J. ANDRES, Palacky University, Faculty of Science, Olomouc, Czech Republic, *Sharkovskii's theorem, differential equations, and beyond*, November 28.
3. F. ATAY, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Stability via time delays: From oscillators to networks*, November 21.
4. J. BALL, Oxford University, Mathematical Institute, UK, *Phase nucleation in solids*, February 24.
5. F. BAUER, Universität Göttingen, Institut für Numerische und Angewandte Mathematik, *The balancing principle — an overview of our current research*, January 10.
6. D. BIMBERG, Technische Universität Berlin, Institut für Festkörperphysik, *Quantum-dot amplifier for 100 Gbit ethernet*, June 13.
7. D. BLÖMKER, RWTH Aachen, Institut für Mathematik, *Stochastic dynamics near a bifurcation – Amplitude equations*, May 17.
8. A. BRADJI, Université de Provence, Centre de Mathématiques et Informatique (CMI), Marseille, France, *Finite volume methods for elliptic problems*, February 15.
9. C. BUTUCEA, Université Paris VI “Pierre et Marie Curie”, Laboratoire de Probabilités et Modèles Aléatoires, France, *New M-estimators in semiparametric regression with errors in variables*, April 19.
10. A. CAPELLA-KORT, Universität Bonn, Institut für Angewandte Mathematik, *On the regularity of stable solutions of semilinear elliptic equations*, May 10.
11. E. CASAS, Universidad de Cantabria, Departamento de Matemática Aplicada y Ciencias de la Computación, Santander, Spain, *Numerical approximation of elliptic control problems with finitely many pointwise state constraints*, April 27.
12. A.R. CHAMPNEYS, University of Bristol, Department of Engineering Mathematics, UK, *Localized patterns*, May 23.
13. K. CHEŁMIŃSKI, Cardinal Stefan Wyszyński University, Faculty for Mathematics and Sciences, Warsaw, Poland, *Elasto-plasticity as a limit of Cosserat plasticity*, July 18.
14. CH. CHONG, San Diego State University, Department of Mathematics, USA, *Multi-stable solitons in the cubic quintic discrete nonlinear Schrödinger equation*, March 14.
15. H. CORNEAN, Aalborg University, Department of Mathematical Sciences, Denmark, *On the zero frequency limit of the Faraday rotation*, November 29.
16. L. DE SANCTIS, International Center for Theoretical Physics, ICTP, Trieste, Italy, *An introduction to rigorous recent results on dilute spin glasses*, May 24.
17. K. DIMOVA, Max-Planck-Institut für Plasmaphysik, Garching, *Modeling the anomalous heat transport in a tokamak plasma. Discontinuity in the derivative of the heat conductivity coefficient*, February 13.
18. F. DITTMAR, Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin, *Stationäre Simulation und experimentelle Charakterisierung von Trapezlasern*, June 29.
19. D. DUNCAN, Heriot–Watt University, School of Mathematical and Computer Sciences, Edinburgh, UK, *Numerical analysis of a convolution model of phase separation*, May 16.
20. M. ELEUTERI, Università degli Studi di Trento, Dipartimento di Matematica, Italy, *Asymptotic behavior of a Neumann parabolic problem with hysteresis*, April 26.
21. M. ESSER, RWTH Aachen, WZL — Laboratorium für Werkzeugmaschinen und Betriebslehre, *Messtechnik und Strukturanalyse an Werkzeugmaschinen*, July 11.

22. R.P. FAASSEN, Technical University Eindhoven, Department of Mechanical Engineering, The Netherlands, *Modelling and detection of machine tool chatter in high speed milling*, November 16.
23. J. FAINBERG, Fraunhofer-Institut für Integrierte Systeme und Bauelementetechnologie, Erlangen, *Konvektion in elektrisch leitenden Fluiden*, March 9.
24. T. FENG, Mid Sweden University, Fibre Science and Communication Network, Sundsvall, Sweden, *Adaptive finite element methods for parameter estimation problems in partial differential equations*, January 9.
25. P. FERRARI, Technische Universität München, Zentrum Mathematik, Bereich M5, *Fluctuations of an atomic ledge bordering a crystalline facet*, July 5.
26. I. FISCHER, Free University of Bruxelles, Department of Applied Physics and Photonics (TONA), Belgium, *Tailored broadband dynamics of an external cavity semiconductor laser and its utilization*, December 7.
27. P. FRATZL, Max-Planck-Institut für Kolloid- und Grenzflächenforschung Potsdam, Abteilung Biomaterialien, *Adaptive Materialien der Natur*, June 19.
28. M. FRIED, Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Angewandte Mathematik, *A level set based adaptive FE algorithm for image segmentation*, March 2.
29. M. GEORGI, Freie Universität Berlin, Institut für Mathematik I, *Interactions of homoclinic solutions and Hopf bifurcations in forward-backward-delay equation*, October 31.
30. K. GLASNER, University of Arizona, Department of Mathematics, Santa Rita, USA, *The role of kinetics-driven migration in coarsening dynamics*, July 11.
31. Y. GOLUBEV, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, *On adaptive methods for inverse estimation*, December 6.
32. L. GRASEDYCK, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Hierarchical matrices based on domain decomposition*, November 2.
33. R.B. GUENTHER, Oregon State University, Mathematics Department, Corvallis, USA, *Penetration of rigid bodies into saturated soils and the response of the soils*, October 17.
34. E. GUERRE, Université Paris VI "Pierre et Marie Curie", Laboratoire de Statistique Théorique et Appliquée, France, *A data-driven nonparametric specification test for dynamic regression models*, June 28.
35. S.M. HASSANIZADEH, Utrecht University, Department of Earth Sciences, The Netherlands, *Modelling flow and transport in industrial porous media*, September 19.
36. D. HILHORST, Université Paris-Sud, Laboratoire d'Analyse Numérique, Orsay, France, *Convergence, a posteriori error estimates, and adaptivity for combined finite volume/finite element schemes on nonmatching grids*, April 25.
37. S. HOCK, Humboldt-Universität zu Berlin, *Discontinuous Galerkin method for elastoplastic problems*, May 3.
38. D. HOFFMANN, Fraunhofer-Institut für Nachrichtentechnik Heinrich-Hertz-Institut (HHI), Berlin, *Hochratige Mach-Zehnder-Interferometer Modulatoren: Aktuelle Ergebnisse und zukünftige Herausforderungen*, April 3.
39. P. HÖVEL, S. SCHIKORA, Technische Universität Berlin, Institut für Theoretische Physik, und Humboldt-Universität zu Berlin, Institut für Physik, *All-optical noninvasive control of unstable steady states in a semiconductor laser*, July 6.
40. O. HOVORKA, Drexel University, College of Engineering, Philadelphia, USA, *Rate independent effect in systems with scalar hysteresis*, October 10.
41. G.C. HSIAO, University of Delaware, Department of Mathematical Sciences, Newark, USA, *On a fluid-structure interaction problem in scattering*, July 18.
42. F. JELTSCH, Universität Potsdam, Institut für Biochemie und Biologie, *Simulating savanna dynamics: From system stability to biodiversity*, May 29.

43. A. JUDITSKY, Université Joseph Fourier Grenoble I, Laboratoire de Modélisation et Calcul, France, *Statistical inference for large-scale resource allocation problem*, January 4.
44. S.A. KASCHENKO, Yaroslavl State University, Department of Mathematical Modeling, Russia, *Asymptotic methods for nonlinear systems with time delay*, September 21.
45. A. KHLUDNEV, Russian Academy of Sciences, Lavrentyev Institute of Hydrodynamics, Novosibirsk, *Crack problems in solid mechanics with possible contact between crack faces*, January 17.
46. E. KHRUSLOV, B. Verkin Institute for Low Temperature Physics and Engineering (ILTPE), Kharkov, Ukraine, *Homogenization problems of Riemannian models with complicated microstructure*, October 25.
47. D. KLATTE, University of Zurich, Institute of Operations Research, Switzerland, *Lipschitz-Stabilität stationärer Lösungen von nichtlinearen Optimierungsproblemen*, January 3.
48. E. KNOBLOCH, University of California, Department of Physics, Berkeley, USA, *Localized patterns*, May 23.
49. A. KOROL, University of Haifa, Institute of Evolution, Israel, *Mapping the genome: Mathematical and computational challenges*, October 16.
50. E. KOROTYAEV, Humboldt-Universität zu Berlin, Institut für Mathematik, *Spectral estimates for 1D Schrödinger operators with periodic potentials*, November 7.
51. TH. KRIECHERBAUER, Ruhr-Universität Bochum, Fakultät für Mathematik, *Analyzing the Toda lattice using integrability*, March 21.
52. J. KRISTENSEN, University of Oxford, Mathematical Institute, UK, *Examples of quasiconvex functions*, May 17.
53. ———, *On the regularity of minimizers of multiple integrals*, June 7.
54. K. KRUMBIEGEL, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, *Feasible iterative methods – error estimates and numerical treatment*, August 1.
55. K. KUHNEN, Universität des Saarlandes, Physik und Mechatronik, Saarbrücken, *Neue Steuerungskonzepte für mechatronische Systeme mit aktiven Materialien (Am Beispiel eines piezoelektrischen Positioniersystems mit paralleler Kinematik)*, April 11.
56. ———, *FPGA-based inverse filter design for the compensation of hysteretic nonlinearities in high-speed applications*, November 21.
57. F. LEGOLL, École Nationale des Ponts et Chaussées, Laboratoire d'Analyse des Matériaux et Identification, Marne-la-Vallée, France, *Multiscale methods coupling atomistic and continuum mechanics: Analysis of a simple case*, December 11.
58. M. LICHTNER, Humboldt-Universität zu Berlin, Institut für Mathematik, *A spectral gap mapping theorem and smooth invariant manifolds for semilinear hyperbolic systems*, January 17.
59. A. LINKE, DFG Research Center MATHEON, Berlin, *Computing incompressible flows by stabilized lowest-order Scott–Vogelius elements*, March 23.
60. A. LORENT, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *An L^p two-well theorem and applications*, July 12.
61. G. LUBE, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik (NAM), *Stabilized FEM for incompressible flows. A critical review and new trends*, January 18.
62. M.G. LÜLING, Schlumberger Paris, France, *Underground storage to clean the atmosphere*, May 8.
63. Z. MACZYNSKA, RWTH Aachen, Institut für Mathematik, *Rigorous numerics for heteroclinic connections*, December 5.
64. M.M. MALAMUD, Donetsk National University, Department of Mathematics, Ukraine, *Completeness of root vectors for nonselfadjoint Sturm–Liouville operators with arbitrary boundary conditions*, December 12.

65. J.A. MARTINS, Instituto Superior Técnico, Departamento de Engenharia Civil, Lisboa, Portugal, *Finite element studies of the deformation of skeletal muscles*, October 18.
66. F. MÉHATS, Université de Rennes 1, Institut de Recherche Mathématique de Rennes (IRMAR), France, *Quantum hydrodynamics models based on the maximum entropy principle*, May 10.
67. L.A. MELNIKOV, Saratov State University, Department of Laser and Computer Physics, Russia, *Vectorial Karhunen–Loeve modes for the description of the polarization transverse pattern dynamics in lasers and classification of the vector singular points*, September 19.
68. D. MERKT, Brandenburgische Technische Universität Cottbus, Lehrstuhl für Theoretische Physik, *Spatiotemporal evolution of bounded two-layer films in lubrication approximation*, February 7.
69. G.R. MINGIONE, Università degli Studi di Parma, Dipartimento di Matematica, Italy, *Calderon–Zygmund estimates for degenerate parabolic systems*, April 19.
70. N. MOELANS, Catholic University of Leuven, Department of Metallurgy and Materials Engineering, Belgium, *Phase-field simulations of grain growth in materials containing second-phase particles*, June 7.
71. C. MUELLER, University of Rochester, Department of Mathematics, USA, *The speed of a random traveling wave*, July 19.
72. N. NATARAJ, Indian Institute of Technology, Department of Mathematics, Bombay, *Mixed finite element methods for fourth-order problems*, May 24.
73. S. NEČASOVÁ, Academy of Sciences of the Czech Republic, Mathematical Institute, Prague, *An L^p approach of viscous fluid flow past a rotating obstacle*, November 22.
74. P. NEFF, Technische Universität Darmstadt, Fachbereich Mathematik, *A numerical solution method for an infinitesimal elasto-plastic Cosserat model*, November 8.
75. S. NESENEKO, Technische Universität Darmstadt, Fachbereich Mathematik, *Homogenization and regularity in viscoplasticity*, July 26.
76. F. NIER, Université de Rennes 1, Institut de Recherche Mathématique de Rennes (IRMAR), France, *Resonant tunneling diodes: Modelling, results and mathematical issues*, November 1.
77. M. NIZETTE, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, *The Q-switching instability in passively mode-locked lasers*, November 7.
78. F. ORTEGON GALLEGO, Universidad de Cadiz, Departamento de Matemáticas, Puerto Real, Spain, *The thermistor problem under the Wiedemann–Franz law and metallic conduction*, September 5.
79. J. OUTRATA, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, *On the control of an evolutionary equilibrium in magnetism*, February 28.
80. ———, *Sharp necessary optimality conditions in control of contact problems with strings*, December 19.
81. C. PATZ, CERMICS, Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée, France, *Dispersive and long-time behavior of oscillations in lattices*, March 30.
82. A. PETROV, Université Claude Bernard (Lyon I), Laboratoire MAPLY, France, *Some results on the stability of quasi-static paths of elastic-plastic systems with hardening*, June 16.
83. V. PETZET, Universität Bayreuth, Lehrstuhl für Ingenieurmathematik, *Mathematische Modellierung der Heißrissbildung beim Laserschweißen von Aluminium*, February 23.
84. P. PHILIP, University of Minnesota, Institute for Mathematics and its Applications, Minneapolis, USA, *A quasistatic crack propagation model allowing for cohesive forces and crack reversibility*, July 10.
85. M. PIETRZYK, Berlin, *How to describe ultrashort pulse propagation when the NSE does not apply*, November 9.
86. D. POLISEVSKI, Romanian Academy, Institute of Mathematics “Simion Stoilov”, Bucharest, *Asymptotic thermal flow around a highly conductive suspension*, January 11.

87. U. PRAHL, RWTH Aachen, Institut für Eisenhüttenkunde, *Thermodynamik und Kinetik der Phasenumwandlung in Stahl*, November 8.
88. A. RADEMACHER, Universität Dortmund, Fachbereich Mathematik, *Finite element discretization of dynamic contact problems*, April 4.
89. L. RECKE, Humboldt-Universität zu Berlin, Institut für Mathematik, *On eigenvalues and stability related to the travelling wave model*, January 12.
90. ———, *On the concept of rotating and modulated wave solutions*, October 19.
91. W. RING, Karl-Franzens-Universität Graz, Institut für Mathematik, Austria, *Level set based shape optimization techniques*, August 24.
92. Y. RITOV, The Hebrew University of Jerusalem, Department of Statistics, Israel, *LASSO regression, persistence and model selection*, October 18.
93. E. ROCCA, Università degli Studi di Milano, Dipartimento di Matematica “F. Enriques”, Italy, *A dual formulation for a class of phase-field systems: Existence and long-time behaviour of solutions*, October 25.
94. A. ROLO NARANJO, Instituto Superior de Tecnologías y Ciencias Aplicadas, Havana, Cuba, *Computational tools for signal processing applications from industry and bioinformatics*, February 6.
95. N. ROSANOV, Institute for Laser Physics, St. Petersburg, Russia, *Laser solitons and their motion*, January 19.
96. J. ROSSMANN, Universität Rostock, Institut für Mathematik, *Regularitätsaussagen für Lösungen elliptischer Randwertaufgaben in Polyedergebieten*, July 5.
97. I. RUBINSTEIN, Ben-Gurion University of the Negev, The Jacob Blaustein Institute for Desert Research, Sede Boquer Campus, Israel, *From equilibrium to non-equilibrium electric double layer, electro-osmosis and electro-convective instability of electric conduction from an electrolyte solution into a charge selective solid*, February 16.
98. A. SAKAI, EURANDOM, Eindhoven, The Netherlands, *Lace expansion for the Ising model*, January 25.
99. S. SAUTER, Universität Zürich, Institut für Mathematik, Switzerland, *Helmholtz-Gleichung und ein neuer Zugang zur Konvergenztheorie*, December 12.
100. A. SCHEEL, University of Minnesota, School of Mathematics, Minneapolis, MN, USA, *Periodic patterns: Modulations, bifurcations, and perturbations*, April 6.
101. A. SCHLIWA, Technische Universität Berlin, Institut für Festkörperphysik, *Das 8-band k.p Modell und die Konfigurations-Wechselwirkungs-Methode angewendet auf exzitonische Eigenschaften von InAs/GaAs Quantenpunkten*, November 2.
102. H. SCHULZ-BALDES, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, *Random matrices beyond the Wigner ensemble*, May 24.
103. V. SHCHUKIN, Technische Universität Berlin, Institut für Festkörperphysik, *Novel concepts for high power lasers*, December 21.
104. A. SHISHKOV, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Donetsk, *Evolution of support in multidimensional thin-film flow with nonlinear diffusion, convection and absorption*, July 19.
105. J. SIEBER, University of Bristol, Department of Engineering Mathematics, UK, *Bifurcation tracking with feedback control*, December 12.
106. J. SOKOŁOWSKI, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, *Numerical methods of shape optimization for variational inequalities*, April 11.
107. CH. SPARBER, Universität Wien, Wolfgang Pauli Institut & Fakultät für Mathematik, Austria, *Adiabatic description of piezoelectricity*, September 4.

108. M. SPECIOVIUS-NEUGEBAUER, Universität Kassel, Fachbereich für Mathematik und Informatik, *Artificial boundary conditions for elliptic problems*, April 24.
109. S. SPERLICH, Universidad Carlos III de Madrid, Departamento de Estadística y Econometría, Spain, *Semi-parametric estimation of consumer demand systems in real expenditure with partially linear price effects*, January 11.
110. R. SUN, EURANDOM, Eindhoven, The Netherlands, *Renormalization analysis of hierarchically interacting two-type branching model*, February 8.
111. I. SUSHKO, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, *Dynamics of 2D border collision normal form*, December 21.
112. R. SZALAI, University of Bristol, Department of Engineering Mathematics, UK, *Dynamics of milling processes*, November 14.
113. K. THEISSEN, Universität Münster, Institut für Numerische und Angewandte Mathematik, *Controlling non-linear evolution equations into stationary solutions*, April 6.
114. M. THERA, Université de Limoges, Laboratoire d'Arithmétique, de Calcul Formel et d'Optimisation, France, *Boundary half-strips and the strong CHIP*, June 14.
115. D. TIBA, Romanian Academy, Institute of Mathematics, Bucharest, *The control variational method*, February 7.
116. ———, *The control variational method*, November 8.
117. U. TROPPE, Fraunhofer-Institut für Nachrichtentechnik Heinrich-Hertz-Institut (HHI), Berlin, *Passive feedback laser structures with high modulation bandwidth: Theory and experiment*, June 22.
118. S. TSENG, Tamkang University, Department of Mathematics, Tamsui, Taiwan, *A stochastic analysis on dynamic biological systems*, July 18.
119. D. TURAEV, Ben Gurion University of the Negev, Department of Mathematics, Beer Sheva, Israel, *On the complex Lorenz attractor*, July 18.
120. S. VAN DE GEER, Eidgenössische Technische Hochschule Zürich, Institut für Mathematik, Switzerland, *The LASSO as an oracle*, February 8.
121. I. VAN KEILEGOM, Université Catholique de Louvain, Institut de Statistique, Louvain-la-Neuve, Belgium, *Estimation of a semiparametric transformation model*, July 5.
122. B. VEXLER, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, *Adaptive space-time finite elements for parabolic optimization problems*, June 21.
123. C. VIAL, Université Paris X, Laboratoire Modal'X, Nanterre, France, *Local model selection in inverse problem*, May 31.
124. M. WAGNER, Brandenburgische Technische Universität Cottbus, Institut für Mathematik, *Multidimensional control problems in image processing*, April 26.
125. A. WAKOLBINGER, Johann Wolfgang Goethe-Universität Frankfurt, Institut für Stochastik und Mathematische Informatik, *Most recent common ancestors in an evolving coalescent: How they come and how they go*, July 12.
126. H. WENZEL, Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin, *On model equations for lasers with tapered sections*, November 23.
127. M. WOLF, Universität Zürich, Institut für Empirische Wirtschaftsforschung, Switzerland, *Formalized data snooping based on generalized error rates*, June 14.
128. M. YAMAMOTO, University of Tokyo, Department of Mathematical Sciences, Japan, *Asymptotic behaviour of Tikhonov regularized solutions and application to the image edge detection*, April 13.
129. ———, *Stability analysis for state estimation problems for heat processes — backward heat problem and inverse heat conduction problem*, September 21.

- 130. X. YAO, Tsinghua University, Beijing, PR China, *Random graph and complex networks*, July 3.
- 131. V.A. ZAGREBNOV, Université Aix-Marseille II, Centre de Physique Théorique, France, *Mechanical instability of semiconductors: Metal-exciton isolator transitions*, May 2.
- 132. S. ZELIK, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, *Multipulses and space-time chaos in dissipative systems*, January 17.
- 133. ———, *Spatially nondecaying solutions of 2D Navier–Stokes equations in a strip*, May 3.
- 134. ———, *Global attractors for 2D Navier–Stokes equations in a strip in the class of spatially non-decaying solutions*, June 27.
- 135. ———, *Interaction of solitons in dissipative systems*, July 3.
- 136. G. ZHANG, Philips Semiconductors, Eindhoven, and Delft University of Technology, Department of Precision and Manufacturing Engineering, The Netherlands, *Some trends and impacts of micro/nanoelectronics*, January 23.
- 137. H. ZHAO, Freie Universität Berlin, Fachbereich Mathematik und Informatik, *Model reduction in single mirror feedback systems*, February 17.
- 138. D. ZHENG, Continental AG, Hannover, *Tire FEM simulation at Continental AG*, January 16.

A.14 Software

adimpro (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: tabelow@wias-berlin.de)

adimpro is a contributed package within the R-Project for Statistical Computing that contains tools to perform adaptive smoothing of digital images and some more basic image processing tools. Binaries for several operating systems are available from the Comprehensive R Archive Network (<http://cran.r-project.org>).

AWS (contact: J. Polzehl, phone: +49 30/20372-481, e-mail: polzehl@wias-berlin.de)

AWS is a contributed package within the R-Project for Statistical Computing that contains a reference implementation of the adaptive weights smoothing algorithms for local constant likelihood and local polynomial regression models. Binaries for several operating systems are available from the Comprehensive R Archive Network (<http://cran.r-project.org>).

BOP (contact: J. Borchardt, phone: +49 30/20372-485, e-mail: borchardt@wias-berlin.de)

The simulator **BOP** (**B**lock **O**rientend **P**rocess simulator) is a software package for large-scale process simulation. It allows to solve dynamic as well as steady-state problems and enables Monte Carlo simulations. Due to an equation-based approach, a wide range of processes as they occur in chemical process industries or other process engineering environments can be simulated.

The modeling language of **BOP** is a high-level language that supports a hierarchically unit-oriented description of the process model and enables a simulation concept that is based on a divide-and-conquer strategy. Exploiting this hierarchical modeling structure, the generated system of coupled differential and algebraic equations (DAEs) is partitioned into blocks, which can be treated almost concurrently. The numerical methods used are especially adopted for solving large-scale problems on parallel computers. They include backward differentiation formulae (BDF), block-structured Newton-type methods, and sparse matrix techniques.

BOP is implemented under UNIX on parallel computers with shared memory, but can also be run efficiently on different single processor machines, as well as under LINUX or Windows XP. So far it has been successfully used for the simulation of several real-life processes in heat-integrated distillation, sewage sludge combustion, or catalytic CO oxidation in automotive oxygen sensors, for example. Currently, it is commercially used for gas turbine simulation.

Detailed information: <http://www.wias-berlin.de/software/BOP>

ClusCorr98[®] (contact: H.-J. Mucha, phone: +49 30/20372-573, e-mail: mucha@wias-berlin.de)

The statistical software **ClusCorr98**[®] is an interactive statistical computing environment with the main focus on clustering techniques. A highlight is the automatic validation technique of cluster analysis results performed by a general built-in validation tool that is based on resampling techniques. For example, the automatic validation of hierarchical clustering can be considered as a three-level assessment of stability. The first and most general level is decision-making about the appropriate number of clusters. The decision is based on such well-known measures of correspondence between partitions like the Rand index, the adjusted Rand index, and the index of Fowlkes and Mallows. Second, the stability of each individual cluster is assessed based on measures of similarity between sets, e.g., the asymmetric measure of cluster agreement or the symmetric Jaccard measure. It does make sense to investigate the (often quite different) specific stability of clusters.

In the third and most detailed level of validation, the reliability of the cluster membership of each individual observation can be assessed.

ClusCorr98[®] performs exploratory data analysis mainly by using adaptive methods of cluster analysis, classification, and multivariate visualization. The main focus here is on simple stable models accompanied by appropriate multivariate (graphical) methods like principal components plots and informative dendrograms (binary trees). Usually, the performance and stability of these methods can be improved by using them in a local and adaptive local fashion.

ClusCorr98[®] uses the Excel spreadsheet environment and its database connectivity. The programming language is Visual Basic for Applications (VBA).

Further information: <http://www.wias-berlin.de/software/ClusCorr98> and <http://www.wias-berlin.de/people/mucha/>

DiPoG (contact: A. Rathsfield, phone: +49 30/20372-457, e-mail: rathsfield@wias-berlin.de)

The program package **DiPoG** (**D**irect and **i**nverse **P**roblems for **o**ptical **G**ratings) provides simulation and optimization tools for periodic diffractive structures with multilayer stacks.

The direct solver computes the field distributions and efficiencies of given gratings for TE and TM polarization as well as under conical mounting for arbitrary polygonal surface profiles. The inverse solver deals with the optimal design of gratings, realizing given optical functions, for example, far-field patterns, efficiency, or phase profiles. The algorithms are based on coupled generalized finite/boundary elements and gradient-type optimization methods.

For detailed information please see <http://www.wias-berlin.de/software/DIPOG>.

gltools (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: fuhrmann@wias-berlin.de)

gltools has been designed with the needs of numerical analysts in mind. Thus, unlike many other packages available, it can be used to enhance existing codes with interactive or non-interactive graphical output. It enhances the OpenGL API with additional functionality allowing to use it for the efficient visualization of time-dependent data on one-, two-, and three-dimensional simplicial grids. Recently, a graphical user interface based on the FLTK toolkit has been added to the package.

Please find further information under <http://www.wias-berlin.de/software/gltools>.

fmri (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: tabelow@wias-berlin.de)

fmri is a contributed package within the R-Project for Statistical Computing that contains tools to analyze fMRI data with structure adaptive smoothing procedures. Binaries for several operating systems are available from the Comprehensive R Archive Network (<http://cran.r-project.org>).

LDL-tool (contact: M. Radziunas, phone: +49 30/20372-441, e-mail: radziunas@wias-berlin.de)

LDL-tool (**L**ongitudinal **D**ynamics in **S**emiconductor **L**asers) is a tool for the simulation and analysis of the nonlinear longitudinal dynamics in multi-section semiconductor lasers and different coupled laser devices. This software is used to investigate and to design laser devices that exhibit various nonlinear effects such as self-pulsations, chaos, hysteresis, mode switching, excitability, mutual synchronization and frequency entrainment by an external modulated optical or electrical signal.

`LDL-tool` combines models of different complexity, ranging from partial differential equation (PDE) to ordinary differential equation (ODE) systems. A mode analysis of the PDE system, a comparison of the different models, and a numerical bifurcation analysis of PDE systems are also possible.

Detailed information: <http://www.wias-berlin.de/software/ldsl>

pdelib (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: fuhrmann@wias-berlin.de)

`pdelib` is a collection of software components that are useful to create simulators based on partial differential equations. The main idea of the package is modularity, based on a bottom-up design realized in the C++ programming language. Among others, it provides libraries for

- iterative solvers
- sparse matrix structures with preconditioners and direct solver interfaces
- simplex grid handling
- parallelization on SMP architectures
- graphical output using `gltools` and OpenGL
- user interface based on the scripting language Lua
- graphical user interface based on the FLTK toolkit

Further, based on the finite volume implicit Euler method, a solver for systems of nonlinear reaction-diffusion-convection equations in heterogeneous one-, two-, and three-dimensional domains has been implemented that is part of the package.

For more information please see also <http://www.wias-berlin.de/software/pdelib>.

WIAS-3dReduce (contact: I. Bremer, phone: +49 30/20372-315, e-mail: bremer@wias-berlin.de)

Based on SGI's OpenGL Performer and COG, this is a software for optimizing the visualization performance of 3D objects in a virtual reality environment. It reduces the number of surface vertices and triangles with or without changing the visible geometry. Automatic level-of-detail generation is included. Many 3D formats are supported through Performer loader plugins, especially VRML, Open Inventor, and Relax. The package is distributed as part of Rücker Factory Invision by Rücker EKS GmbH (holger.haemmerle@ruecker.de) under the name `rfreduce`.

WIAS-HITNIHS (contact: O. Klein, phone: +49 30/20372-533, e-mail: klein@wias-berlin.de)

The **WIAS-High Temperature Numerical Induction Heating Simulator** constitutes a transient simulation tool for the temperature evolution in axisymmetric technical systems that are subject to intense heating by induction. The simulator accounts for heat transfer by radiation through cavities, and it allows for changes in the material parameters due to the rising temperature and for some kinds of anisotropy within the thermal conductivity.

The simulator is designed to deal with complicated axisymmetric setups having a polygonal 2D projection. The software is based on the WIAS program package `pdelib` for the numerical solution of partial differential equations and has a graphical user interface provided by `WIAS-MatConE`.

`WIAS-HITNIHS` is further developed within the project “*Numerical simulation and control of sublimation growth of semiconductor bulk single crystals*” supported by DFG (since 2002).

Please find further information under <http://www.wias-berlin.de/software/hitnihs>.

WIAS-MatConE (contact: O. Klein, phone: +49 30/20372-533, klein@wias-berlin.de)

The WIAS-**Material** data file and **Control** file **Edit** GUI is a software tool to provide prototypical graphical user interfaces (GUIs) for creating and editing files that are used as inputs for simulation software, like, for example, material data and control files.

The contents of a file type to be considered are described by a list of input requests for real numbers, integer numbers, strings, file names, fields of real numbers, and fields of real vectors, which are combined with comments, information about units, pictures, and further structural information, like, for example, the information that the settings for the time step control need only be requested for transient problems. Using this list, WIAS-MatConE allows to create and edit the considered type of file within a GUI framework.

WIAS-MatConE provides a fast and flexible way to generate GUIs for prototypical software without having to deal with the details of GUI development.

WIAS-SHarP (contact: W. Weiss, phone: +49 30/20372-478, e-mail: weiss@wias-berlin.de)

Based on `pdelib`, WIAS-SHarP (**S**urface **H**ardening **P**rogram) is a software for the simulation of electron and laser beam surface hardening. It contains a data bank with material parameters for 20 important steels as well as routines to describe the phase transition kinetics during one heat treatment cycle. Moreover, it allows for an easy implementation of different radiation flux profiles. In the new version, an adaptive grid is used. To facilitate its usage, a Java-based GUI has been developed.

For more information see <http://www.wias-berlin.de/software/sharp>.

WIAS-TeSCA (contact: R. Nürnberg, phone: +49 30/20372-570, e-mail: nuernberg@wias-berlin.de)

WIAS-TeSCA is a **Two-** and **three-dimensional Semi-Conductor Analysis** package. It serves to simulate numerically the charge carrier transport in semiconductor devices based upon the drift-diffusion model. This van Roosbroeck system is augmented by a vast variety of additional physical phenomena playing a role in the operation of specialized semiconductor devices, as, e.g., the influence of magnetic fields, optical radiation, temperature, or the kinetics of deep (trapped) impurities.

The strategy of WIAS-TeSCA for solving the resulting highly nonlinear system of partial differential equations is oriented towards the Lyapunov structure of the system that describes the currents of electrons and holes within the device. Thus, efficient numerical procedures, for both the stationary and the transient simulation, have been implemented, the spatial structure of which is a finite volume method. The underlying finite element discretization allows the simulation of arbitrarily shaped two-dimensional device structures.

WIAS-TeSCA has been successfully used in the research and development of semiconductor devices such as transistors, diodes, sensors, detectors, and lasers.

The semiconductor device simulation package WIAS-TeSCA operates in a UNIX environment and is available for a variety of configurations as, e.g., SUN, COMPAQ, but also for Linux PC.

For more information please see <http://www.wias-berlin.de/software/tesca>.

WIAS-QW (contact: Th. Koprucki, phone: +49 30/20372-508, e-mail: koprucki@wias-berlin.de)

WIAS-QW is a numerical code for the simulation of strained multi-quantum-well structures. Based upon multi-band kp models it allows to treat band mixing effects, confinement effects, crystal symmetry, and the influence of mechanical strain.

In particular, **WIAS-QW** calculates the

- subband dispersion
- eigenfunctions
- transition matrix elements
- miniband effects in multi-quantum-well structures

In dependence on the sheet carrier densities and the temperature, **WIAS-QW** calculates the

- optical response function
- gain spectrum
- radiative recombination rate
- carrier density distributions

Furthermore, the calculations can be done selfconsistently, comprising pure *kp* calculations, but also calculations that include the Hartree–Coulomb potential, obtained from Poisson’s equation, as well as density-dependent exchange-correlation potentials accounting for the bandgap-shift, which is one of the most prominent many-particle effects.

Please find further information under <http://www.wias-berlin.de/software/qw>.